

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSPTAJRK1626

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

\* \* \* \* \* Welcome to STN International \* \* \* \* \*

NEWS	1		Web Page for STN Seminar Schedule - N. America
NEWS	2	AUG 15	CAOLD to be discontinued on December 31, 2008
NEWS	3	OCT 07	EPFULL enhanced with full implementation of EPC2000
NEWS	4	OCT 07	Multiple databases enhanced for more flexible patent number searching
NEWS	5	OCT 22	Current-awareness alert (SDI) setup and editing enhanced
NEWS	6	OCT 22	WPIDS, WPINDEX, and WPIX enhanced with Canadian PCT Applications
NEWS	7	OCT 24	CHEMLIST enhanced with intermediate list of pre-registered REACH substances
NEWS	8	NOV 21	CAS patent coverage to include exemplified prophetic substances identified in English-, French-, German-, and Japanese-language basic patents from 2004-present
NEWS	9	NOV 26	MARPAT enhanced with FSORT command
NEWS	10	NOV 26	MEDLINE year-end processing temporarily halts availability of new fully-indexed citations
NEWS	11	NOV 26	CHEMSAFE now available on STN Easy
NEWS	12	NOV 26	Two new SET commands increase convenience of STN searching
NEWS	13	DEC 01	ChemPort single article sales feature unavailable
NEWS	14	DEC 12	GBFULL now offers single source for full-text coverage of complete UK patent families
NEWS	15	DEC 17	Fifty-one pharmaceutical ingredients added to PS
NEWS EXPRESS	JUNE 27 08 CURRENT WINDOWS VERSION IS V8.3, AND CURRENT DISCOVER FILE IS DATED 23 JUNE 2008.		
NEWS HOURS	STN Operating Hours Plus Help Desk Availability		
NEWS LOGIN	Welcome Banner and News Items		
NEWS IPC8	For general information regarding STN implementation of IPC 8		

Enter NEWS followed by the item number or name to see news on that specific topic.

All use of STN is subject to the provisions of the STN Customer agreement. Please note that this agreement limits use to scientific research. Use for software development or design or implementation of commercial gateways or other similar uses is prohibited and may result in loss of user privileges and other penalties.

\* \* \* \* \* STN Columbus \* \* \* \* \*

FILE 'HOME' ENTERED AT 10:37:11 ON 19 DEC 2008

=> file reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'REGISTRY' ENTERED AT 10:37:23 ON 19 DEC 2008

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

COPYRIGHT (C) 2008 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 17 DEC 2008 HIGHEST RN 1086212-50-1

DICTIONARY FILE UPDATES: 17 DEC 2008 HIGHEST RN 1086212-50-1

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH July 5, 2008.

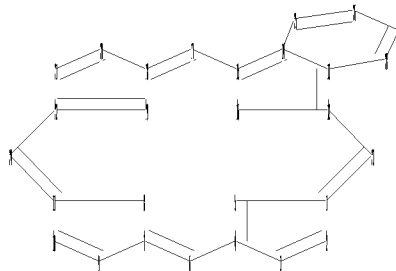
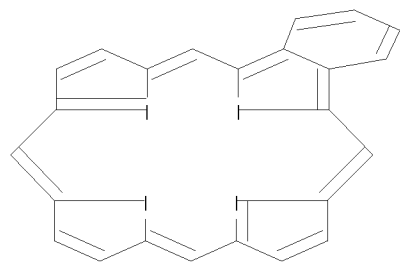
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10583126\Struc 1.str



ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23  
24 25 26 27 28

ring bonds :

1-2 1-5 1-23 2-3 3-4 4-5 4-6 6-7 7-8 7-9 8-11 9-10 10-11 11-24 12-13  
12-16 12-23 13-14 13-28 14-15 14-25 15-16 15-17 17-18 18-19 18-20 19-22  
20-21 21-22 22-24 25-26 26-27 27-28

exact/norm bonds :

7-8 8-11 12-16 15-16

normalized bonds :

10583126.trn

1-2 1-5 1-23 2-3 3-4 4-5 4-6 6-7 7-9 9-10 10-11 11-24 12-13 12-23  
 13-14 13-28 14-15 14-25 15-17 17-18 18-19 18-20 19-22 20-21 21-22 22-24  
 25-26 26-27 27-28

Match level :

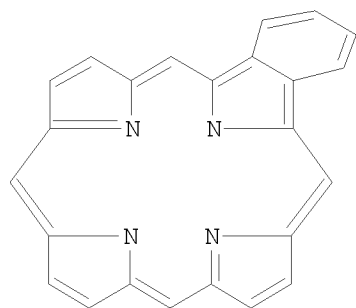
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom  
 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom  
 20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom

L1 STRUCTURE UPLOADED

=> d

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> l1

SAMPLE SEARCH INITIATED 10:37:45 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 799 TO ITERATE

100.0% PROCESSED 799 ITERATIONS

50 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 14285 TO 17675

PROJECTED ANSWERS: 849 TO 1831

L2 50 SEA SSS SAM L1

=> l1 full

FULL SEARCH INITIATED 10:37:50 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 15629 TO ITERATE

100.0% PROCESSED 15629 ITERATIONS

1509 ANSWERS

SEARCH TIME: 00.00.01

10583126.trn

L3 1509 SEA SSS FUL L1

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	178.36	178.57

FILE 'CAPLUS' ENTERED AT 10:37:53 ON 19 DEC 2008  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
COPYRIGHT (C) 2008 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 19 Dec 2008 VOL 149 ISS 26  
FILE LAST UPDATED: 18 Dec 2008 (20081218/ED)

Caplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2008.

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

<http://www.cas.org/legal/infopolicy.html>

=> 13

L4 948 L3

=> 14 and transistor

111724 TRANSISTOR

L5 26 L4 AND TRANSISTOR

=> d ibib abs hitstr 1-26

L5 ANSWER 1 OF 26 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2008:1304565 CAPLUS

DOCUMENT NUMBER: 149:502692

TITLE: Organic electroluminescence devices and their displays

INVENTOR(S): Yoshida, Hidehiro; Kanegae, Arinobu; Nakaya, Shuhei;  
Omae, Hideki

PATENT ASSIGNEE(S): Matsushita Electric Industrial Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 13pp.

CODEN: JKXXAF

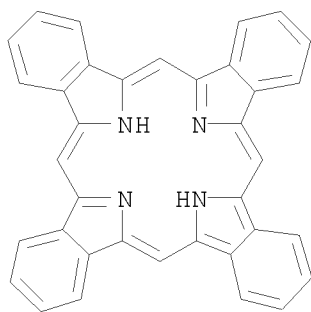
DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	JP 2008261954	A	20081030	JP 2007-103238	20070410
PRIORITY APPLN. INFO.:				JP 2007-103238	20070410
AB	Title devices have pixel electrodes laminated with source or drain electrodes of transistors. Are also claimed, the devices having organic luminescence transistors and transistors for switches. Because the laminated structures decrease area of the transistors, high aperture ratio is achieved, providing flexible displays.				
IT	52952-31-5, Tetrabenzoporphyrin RL: TEM (Technical or engineered material use); USES (Uses) (gate electrode; flexible high-aperture-ratio organic electroluminescence displays having pixel electrodes laminated with transistor electrodes)				
RN	52952-31-5 CAPLUS				
CN	29H,31H-Tetrabenzob[b,g,l,q]porphine (CA INDEX NAME)				



L5 ANSWER 2 OF 26 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2008:1279269 CAPLUS  
 DOCUMENT NUMBER: 149:460807  
 TITLE: Organic thin film transistor and its manufacture by printing  
 INVENTOR(S): Miyai, Mitsuyoshi  
 PATENT ASSIGNEE(S): Konica Minolta Holdings, Inc., Japan  
 SOURCE: Jpn. Kokai Tokkyo Koho, 16pp.  
 CODEN: JKXXAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	JP 2008258252	A	20081023	JP 2007-96183	20070402
PRIORITY APPLN. INFO.:				JP 2007-96183	20070402
AB	The organic TFT is equipped with a gate electrode, gate insulating layer, source electrode, drain electrode, and organic semiconductor layer formed on a substrate, where the source electrode and/or drain electrode have a porous film of an inorg. conductor in which an organic conductor or organic semiconductor is impregnated. The manufacture process comprises following steps: printing a dispersion solution of the inorg. conductor on the substrate, evaporating a solvent of the solution to form the porous film, printing				

a solution or dispersion of an electrode material to impregnate into the porous film. The organic TFT provides uniform current characteristics and high temperature durability.

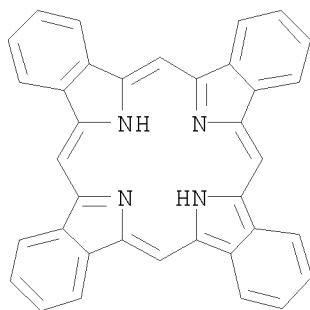
IT 52952-31-5, Tetrabenzoporphyrin

RL: PEP (Physical, engineering or chemical process); TEM (Technical or engineered material use); PROC (Process); USES (Uses)

(organic thin film transistor manufactured by printing on porous inorg. electrode)

RN 52952-31-5 CAPLUS

CN 29H,31H-Tetrabenzob[b,g,l,q]porphine (CA INDEX NAME)



L5 ANSWER 3 OF 26 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2008:1185412 CAPLUS

DOCUMENT NUMBER: 149:437611

TITLE: Process for producing organic transistor and organic transistor

INVENTOR(S): Ohta, Satoru

PATENT ASSIGNEE(S): Pioneer Corporation, Japan

SOURCE: PCT Int. Appl., 21pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2008117450	A1	20081002	WO 2007-JP56425	20070327
<p>W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW</p> <p>RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM</p>				

PRIORITY APPLN. INFO.: WO 2007-JP56425 20070327

AB A process for producing an organic transistor realizing less shift

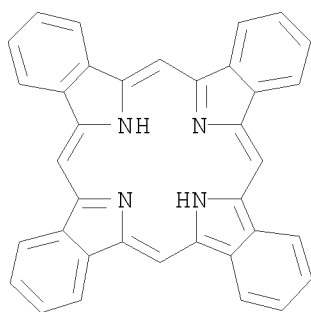
of threshold voltage, including paired source electrode and drain electrode, an organic semiconductor layer for forming a channel between the source electrode and the drain electrode and, laid on the organic semiconductor layer, a gate insulating film and gate electrode, comprises forming a porphyrin compound into a film to form the organic semiconductor layer and simultaneously forming a siloxane compound or silazane compound into a film and hardening the same to give the gate insulating film.

IT 52952-31-5, Tetrabenzoporphyrin

RL: TEM (Technical or engineered material use); USES (Uses)  
(process for producing organic transistor and organic transistor)

RN 52952-31-5 CAPLUS

CN 29H,31H-Tetrabenzob[b,g,l,q]porphine (CA INDEX NAME)



REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 4 OF 26 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2008:626889 CAPLUS

DOCUMENT NUMBER: 149:545947

TITLE: Factors influencing local potential drop in bottom-contact organic thin-film transistor using solution-processible tetrabenzoporphyrin

AUTHOR(S): Xu, Mingsheng; Ohno, Akira; Aramaki, Shinji; Kudo, Kazuhiro; Nakamura, Masakazu

CORPORATE SOURCE: Venture Business Laboratory, Chiba University, 1-33 Yayoi-cho, Inage-ku, Chiba, 263-8522, Japan

SOURCE: Organic Electronics (2008), 9(4), 439-444

CODEN: OERLAU; ISSN: 1566-1199

PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB By exploiting atomic-force-microscope potentiometry, we have studied the local potential distribution in the solution-processible tetrabenzoporphyrin (BP) bottom-contact thin-film transistor under controlled atmospheres. It is found that abrupt and big potential drops mainly appeared at the domain boundaries and cracks in the BP film when the transistor was under operation, indicating a dominant influence of domain boundary and crack on the device performance. Exposure of the device to O<sub>2</sub> drastically reduced the potential drops at some boundaries, which is the main reason for the improved device performance by O<sub>2</sub> exposure.

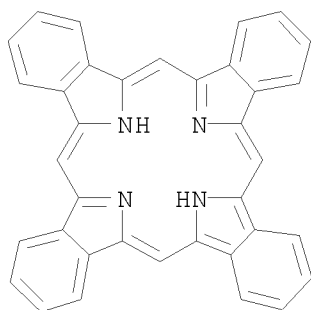
IT 52952-31-5, Tetrabenzoporphyrin

RL: PRP (Properties); TEM (Technical or engineered material use); USES (Uses)

(factors influencing local potential drop in bottom-contact organic thin-film transistor using solution-processible tetrabenzoporphyrin)

RN 52952-31-5 CAPLUS

CN 29H,31H-Tetrabenzob[b,g,l,q]porphine (CA INDEX NAME)



REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 5 OF 26 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2008:190783 CAPLUS

DOCUMENT NUMBER: 148:225814

TITLE: Method for manufacturing a thin film transistor array panel

INVENTOR(S): Shin, Jung-Han; Kim, Bo-Sung; Shin, Seong-Sik

PATENT ASSIGNEE(S): Samsung Electronics Co., Ltd., S. Korea

SOURCE: U.S. Pat. Appl. Publ., 25pp.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20080038867	A1	20080214	US 2007-745722	20070508
KR 2008013297	A	20080213	KR 2006-74638	20060808
PRIORITY APPLN. INFO.:			KR 2006-74638	A 20060808

AB A method of fabricating a thin film transistor array panel is described entailing forming a gate electrode, forming a source electrode and a drain electrode opposing each other and separated from each other on the gate electrode, forming a gate insulator on the gate electrode, forming an organic semiconductor on the gate insulator, and forming a passivation member covering the organic semiconductor, wherein the source and drain electrodes contact the organic semiconductor, and an ink-jet printing process is used to form at least two among the gate insulator, the organic semiconductor, and the passivation member, and wherein a mixed solvent including at least two among a gate insulator material, an organic semiconductor material, and a passivation member material is sprayed in the ink-jet printing process.

IT 52952-31-5, Tetrabenzoporphyrin

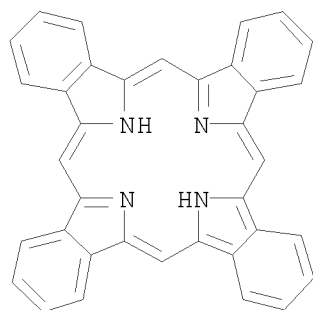
RL: TEM (Technical or engineered material use); USES (Uses)



(organic semiconductor; thin film transistor array panel having organic films formed by simplified ink-jet printing)

RN 52952-31-5 CAPLUS

CN 29H,31H-Tetrabenzo[b,g,l,q]porphine (CA INDEX NAME)



L5 ANSWER 6 OF 26 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2007:1231043 CAPLUS

DOCUMENT NUMBER: 148:89975

TITLE: Metal-insulator transition in solution-processible porphyrinic field-effect transistors

AUTHOR(S): Dhoot, Anoop S.; Aramaki, Shinji; Moses, Daniel; Heeger, Alan J.

CORPORATE SOURCE: Center for Polymers and Organic Solids and Mitsubishi Chemical Center for Advanced Materials, University of California, Santa Barbara, CA, 93106, USA

SOURCE: Advanced Materials (Weinheim, Germany) (2007), 19(19), 2914-2918

CODEN: ADVMEW; ISSN: 0935-9648

PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The charge carrier transport in solution-processible copper tetrabenzoporphyrin field-effect transistors (FETs) was studied and characterized between room temperature and 4.2 K. The insulator-to-metal transition is reached at a carrier d. of  $3 \times 10^{12} \text{ cm}^{-2}$ , approx. independent of the source-drain voltage.

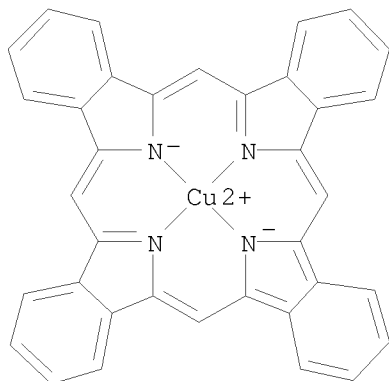
IT 21519-18-6

RL: PRP (Properties)

(metal-insulator transition in solution-processible copper tetrabenzoporphyrin porphyrinic field-effect transistors)

RN 21519-18-6 CAPLUS

CN Copper, [29H,31H-tetrabenzo[b,g,l,q]porphinato(2-)- $\kappa\text{N}29,\kappa\text{N}30,\kappa\text{N}31,\kappa\text{N}32$ ]-, (SP-4-1)- (CA INDEX NAME)



REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 7 OF 26 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2007:688417 CAPLUS

DOCUMENT NUMBER: 147:155136

TITLE: Polycrystalline tetrabenzoporphyrin organic field-effect transistors with nanostructured channels  
AUTHOR(S): Shea, Patrick B.; Chen, Charlene; Kanicki, Jerzy; Pattison, Lisa R.; Petroff, Pierre; Yamada, Hiroko; Ono, Noboru

CORPORATE SOURCE: Organic and Molecular Electronics Laboratory, Department of Electrical Engineering and Computer Science, The University of Michigan, Ann Arbor, MI, 48109, USA

SOURCE: Applied Physics Letters (2007), 90(23), 233107/1-233107/3

CODEN: APPLAB; ISSN: 0003-6951

PUBLISHER: American Institute of Physics

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Solution-processed organic thin-film field-effect transistors were fabricated using a precursor form of the organic semiconductor tetrabenzoporphyrin (TBP) deposited on a thermal silicon oxide gate insulator patterned with nanometer-scale trenches. Thermal conversion of the precursor film to TBP was enhanced by ordered TBP aggregation in the prepatterned trenches, demonstrating precise control and placement of long- and short-range ordering of the organic semiconductor. Organic thin-film field-effect transistors with channels parallel to trench direction growth were found to have field-effect mobility approaching one order of magnitude greater than transistors fabricated with the channel oriented perpendicular to dendrimer growth.

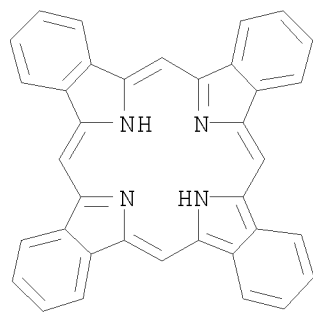
IT 52952-31-5, Tetrabenzoporphyrin

RL: TEM (Technical or engineered material use); USES (Uses)

(fabrication and characteristics of polycryst. tetrabenzoporphyrin organic field-effect transistors with nanostructured channels)

RN 52952-31-5 CAPLUS

CN 29H,31H-Tetrabenzob[b,g,l,q]porphine (CA INDEX NAME)



REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 8 OF 26 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2007:518416 CAPLUS

DOCUMENT NUMBER: 147:155101

TITLE: Solution-processed polycrystalline copper tetrabenzoporphyrin thin-film transistors

AUTHOR(S): Shea, Patrick B.; Pattison, Lisa R.; Kawano, Manami; Chen, Charlene; Chen, Jihua; Petroff, Pierre; Martin, David C.; Yamada, Hiroko; Ono, Noboru; Kanicki, Jerzy  
CORPORATE SOURCE: Organic & Molecular Electronics Laboratory, Department of Electrical Engineering & Computer Science, The University of Michigan, Ann Arbor, MI, 48109-2108, USA

SOURCE: Synthetic Metals (2007), 157(4-5), 190-197

CODEN: SYMEDZ; ISSN: 0379-6779

PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The demonstration of organic thin-film field-effect transistors (OFETs) using a solution-processable form of the organometallic mol. copper tetrabenzoporphyrin (CuTBP) is reported. A soluble precursor was spun-cast into an amorphous, insulating thin-film, and thermally annealed at 165°C for 30 min into a polycryst. organic semiconductor. Absorbance spectroscopy displayed characteristics of porphyrin macrocycles. Microscopy reveals the formation of domains comprising aligned nanorod aggregates with dimensions of 55 nm wide, 300 nm long, and 100 nm tall on the gate insulator surface. OFETs demonstrated field-effect mobilities typically on the order of 0.1 cm<sup>2</sup>/V s, threshold voltages around 5 V, subthreshold slopes around 4 V/dec, and ON-/OFF-current ratios near 10<sup>4</sup>.

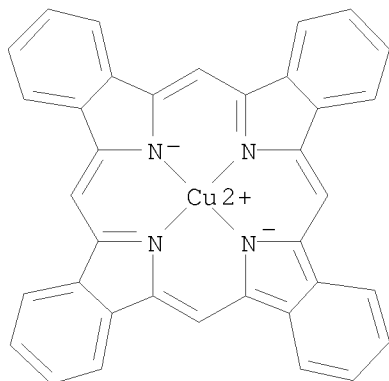
IT 21519-18-6P

RL: PEP (Physical, engineering or chemical process); SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); PROC (Process); USES (Uses)

(solution-processed polycryst. copper tetrabenzoporphyrin thin-film transistors)

RN 21519-18-6 CAPLUS

CN Copper, [29H,31H-tetrabenzo[b,g,l,q]porphinato(2-)-κN29,κN30,κN31,κN32]-, (SP-4-1)- (CA INDEX NAME)



REFERENCE COUNT: 51 THERE ARE 51 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 9 OF 26 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2006:1311691 CAPLUS

DOCUMENT NUMBER: 146:53634

TITLE: Fabrication of organic semiconductor thin film, organic semiconductor thin film, organic electronic device, and organic field-effect transistor

INVENTOR(S): Yoshiyama, Ryuichi; Aramaki, Shinji; Sakai, Yoshitada

PATENT ASSIGNEE(S): Mitsubishi Chemical Corp., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 19pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
-----	----	-----	-----	-----
JP 2006339604	A	20061214	JP 2005-165922	20050606
PRIORITY APPLN. INFO.:			JP 2005-165922	20050606

AB A method for fabricating an organic semiconductor thin film having a large grain size involves preparing an organic semiconductor precursor thin film having a structure for forming a double bond upon a reaction and converting the precursor thin film to a semiconductor thin film while moving a system having a temperature gradient  $d$  ( $^{\circ}\text{C}/\text{mm}$ ) at a moving rate  $x$  ( $\text{mm}/\text{s}$ ) to satisfy an equation  $0.001 < xd < 1000$ .

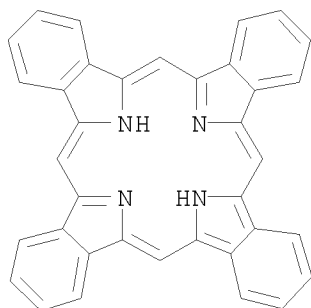
IT 52952-31-5P, 29H,31H-Tetrabenzo[b,g,l,q]porphine

RL: SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

(fabrication of organic semiconductor thin film having large grain size, organic semiconductor thin film, organic electronic device, and organic field-effect transistor)

RN 52952-31-5 CAPLUS

CN 29H,31H-Tetrabenzo[b,g,l,q]porphine (CA INDEX NAME)



L5 ANSWER 10 OF 26 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2006:1012378 CAPLUS

DOCUMENT NUMBER: 145:387605

TITLE: Organic semiconductor device, field-effect transistor, and their manufacturing methods

INVENTOR(S): Nakayama, Tomonari; Ohnishi, Toshinobu; Miura, Daisuke

PATENT ASSIGNEE(S): Canon Kabushiki Kaisha, Japan

SOURCE: U.S. Pat. Appl. Publ., 25pp.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20060214159	A1	20060928	US 2006-373966	20060314
JP 2006303465	A	20061102	JP 2006-75618	20060317
PRIORITY APPLN. INFO.:			JP 2005-88938	A 20050325

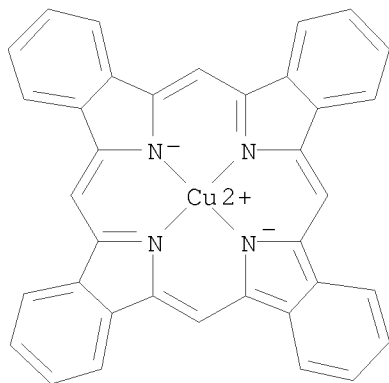
AB An organic semiconductor device is provided which includes an organic semiconductor layer and an insulating layer. The insulating layer is made of a cured material formed from a composition containing a resin and a crosslinking agent. The resin contains an organic resin having a hydroxyl group. The crosslinking agent contains a compound having at least two crosslinking groups. At least one of the crosslinking groups is a methylol group or an NH group. The composition contains the crosslinking agent at 15-45% by weight relative to 100 parts by weight in total of the resin and the crosslinking agent.

IT 21519-18-6 52952-31-5,  
29H,31H-Tetrabenzob[b,g,l,q]porphine  
RL: PRP (Properties); TEM (Technical or engineered material use); USES  
(Uses)

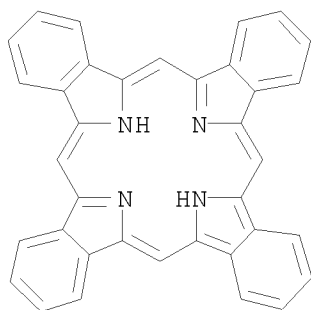
(organic semiconductor device snf field-effect transistor on  
insulating layer substrate)

RN 21519-18-6 CAPLUS

CN Copper, [29H,31H-tetrabenzob[b,g,l,q]porphinato(2-)-  
κN29,κN30,κN31,κN32]-, (SP-4-1)- (CA INDEX NAME)



RN 52952-31-5 CAPLUS  
 CN 29H,31H-Tetrabenzo[b,g,l,q]porphine (CA INDEX NAME)



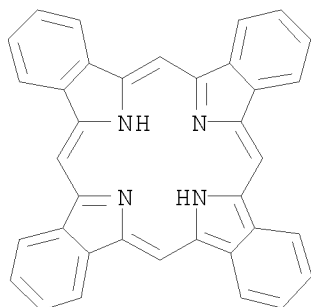
L5 ANSWER 11 OF 26 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2006:949745 CAPLUS  
 DOCUMENT NUMBER: 145:326413  
 TITLE: Manufacture of organic field-effect transistors  
 INVENTOR(S): Aramaki, Shinji; Sakai, Yoshitada; Yoshiyama, Ryuichi  
 PATENT ASSIGNEE(S): Mitsubishi Chemical Corp., Japan  
 SOURCE: Jpn. Kokai Tokkyo Koho, 26pp.  
 CODEN: JKXXAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2006245559	A	20060914	JP 2006-27498	20060203
PRIORITY APPLN. INFO.:			JP 2005-30896	A 20050207

AB The FETs contain, on substrates, organic semiconductor layers from compds. having aza-annulene structure, and mercapto-group-containing layers on  $\geq 1$  side of the semiconductor layers. The FETs have high threshold voltage and excellent ON/OFF ratio.

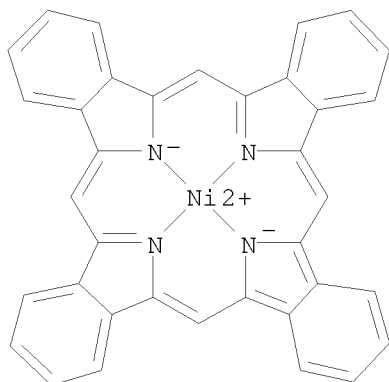
IT 52952-31-5, Tetrabenzoporphyrin

RL: DEV (Device component use); USES (Uses)  
 (manufacture of organic FETs containing semiconductor layers from compds.  
 containing  
 aza-annulene structure)  
 RN 52952-31-5 CAPLUS  
 CN 29H,31H-Tetrabenzo[b,g,l,q]porphine (CA INDEX NAME)

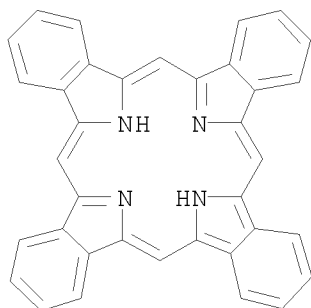


L5 ANSWER 12 OF 26 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2006:839022 CAPLUS  
 DOCUMENT NUMBER: 145:446992  
 TITLE: Solution-processed nickel tetrabenzoporphyrin  
 thin-film transistors  
 AUTHOR(S): Shea, Patrick B.; Kanicki, Jerzy; Pattison, Lisa R.;  
 Petroff, Pierre; Kawano, Manami; Yamada, Hiroko; Ono,  
 Noboru  
 CORPORATE SOURCE: Organic and Molecular Electronics Laboratory,  
 Department of Electrical Engineering and Computer  
 Science, The University of Michigan, Ann Arbor, MI,  
 48109, USA  
 SOURCE: Journal of Applied Physics (2006), 100(3),  
 034502/1-034502/7  
 CODEN: JAPIAU; ISSN: 0021-8979  
 PUBLISHER: American Institute of Physics  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB We describe Ni tetrabenzoporphyrin (NiTBP) as a solution-processible organic  
 semiconductor. Whereas porphyrins in an unmodified state are typically  
 planar and insol., a precursor synthetic route (NiCP) was used to deposit  
 thin films via solution Amorphous, insulating thin films of NiCP were  
 deposited, and thermally converted to polycryst., semiconducting NiTBP.  
 Films were studied using optical absorption and microscopy, atomic force  
 microscopy, and x-ray diffraction. Highly concentrated NiCP was shown to form  
 large, needle-shaped crystals drop-cast from solution NiTBP thin-film  
 field-effect transistors fabricated from spun-cast films demonstrated  
 charge-carrier field-effect mobilities on the order of 0.1 and 0.2 cm<sup>2</sup>/V s  
 and accumulation threshold voltages of -19 and -13, in the linear and  
 saturation regimes, resp.  
 IT 71163-07-0P  
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
 (Ni tetrabenzoporphyrin thin-film transistors)  
 RN 71163-07-0 CAPLUS  
 CN Nickel, [29H,31H-tetrabenzo[b,g,l,q]porphinato(2-)-

κN29, κN30, κN31, κN32]-, (SP-4-1)- (CA INDEX NAME)



IT 52952-31-5, Tetrabenzoporphyrin  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (Ni tetrabenzoporphyrin thin-film transistors)  
 RN 52952-31-5 CAPLUS  
 CN 29H,31H-Tetrabenzo[b,g,l,q]porphine (CA INDEX NAME)

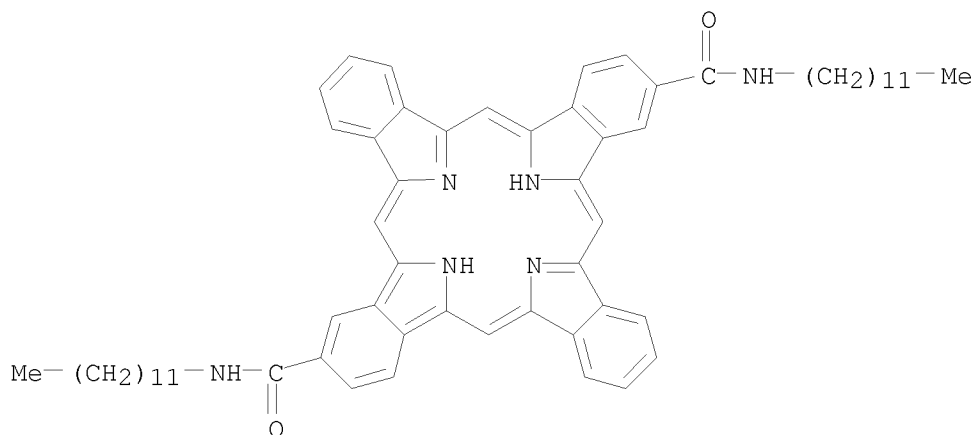


REFERENCE COUNT: 59 THERE ARE 59 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 13 OF 26 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2006:794423 CAPLUS  
 DOCUMENT NUMBER: 145:222853  
 TITLE: Organic semiconductor materials, organic thin film transistors, field-effect transistors (FET), and switching elements  
 INVENTOR(S): Tanaka, Tatsuo  
 PATENT ASSIGNEE(S): Konica Minolta Holdings, Inc., Japan  
 SOURCE: Jpn. Kokai Tokkyo Koho, 30pp.  
 CODEN: JKXXAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:



	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	JP 2006210475	A	20060810	JP 2005-17898	20050126
PRIORITY APPLN. INFO.:				JP 2005-17898	20050126
AB	Organic semiconductors containing compds. having a dye skeleton and that are not				
	organic complexes are claimed. Preferably, the compds. are DRn(D = dye skeleton; R = dissolving unit; n = integer of $\geq 1$ ), (poly)methine dyes, cyanine dyes, merocyanine dyes, oxonol dyes, styryl dyes, (hetero)arylidene dyes, azo dyes, or azomethine dyes. Organic thin film transistors, field-effect transistors (FET), and switching elements comprising the said semiconductors are also claimed. The materials show long service life.				
IT	904665-50-5				
	RL: DEV (Device component use); TEM (Technical or engineered material use); USES (Uses)				
	(organic semiconductors; organic dye semiconductors for TFT, FET, and switching elements)				
RN	904665-50-5	CAPLUS			
CN	29H,31H-Tetrabenzo[b,g,l,q]porphine-2,16-dicarboxamide, N,N'-didodecyl-(9CI) (CA INDEX NAME)				



L5 ANSWER 14 OF 26 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2006:91919 CAPLUS

DOCUMENT NUMBER: 145:387119

TITLE: High performance porphyrin semiconductor for transistor applications

AUTHOR(S): Aramaki, Shinji; Yoshiyama, Ruichi; Sakai, Masayoshi; Ono, Noboru

CORPORATE SOURCE: Mitsubishi Chemical Group Science & Technology Research Center, Inc., 1000 Kamoshida-cho, Aoba-ku, Yokohama, 227-8502, Japan

SOURCE: Digest of Technical Papers - Society for Information Display International Symposium (2005), 36(Bk. 1), 296-299

CODEN: DTPSDS

PUBLISHER: Society for Information Display

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Various porphyrin compds. were investigated for solution-processible semiconductors for transistor applications. Some show excellent semiconductor properties. Their films can be formed by solution-process, i.e., by thermal conversion of their precursor film coated from their solution. Some porphyrin compds. show good semiconductor performance in terms of mobility and long-term driving stability.

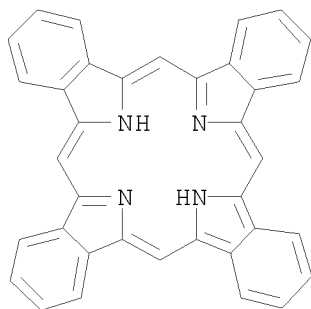
IT 52952-31-5, 29H,31H-Tetrabenzo[b,g,l,q]porphine  
52952-31-5D, 29H,31H-Tetrabenzo[b,g,l,q]porphine, divalent metal complexes 910923-74-9

RL: DEV (Device component use); PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); PROC (Process); USES (Uses)

(high performance porphyrin semiconductor for transistor applications)

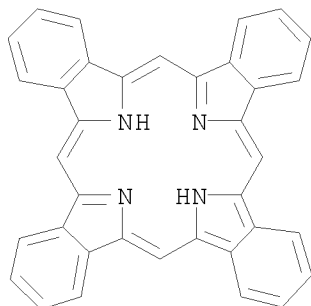
RN 52952-31-5 CAPLUS

CN 29H,31H-Tetrabenzo[b,g,l,q]porphine (CA INDEX NAME)



RN 52952-31-5 CAPLUS

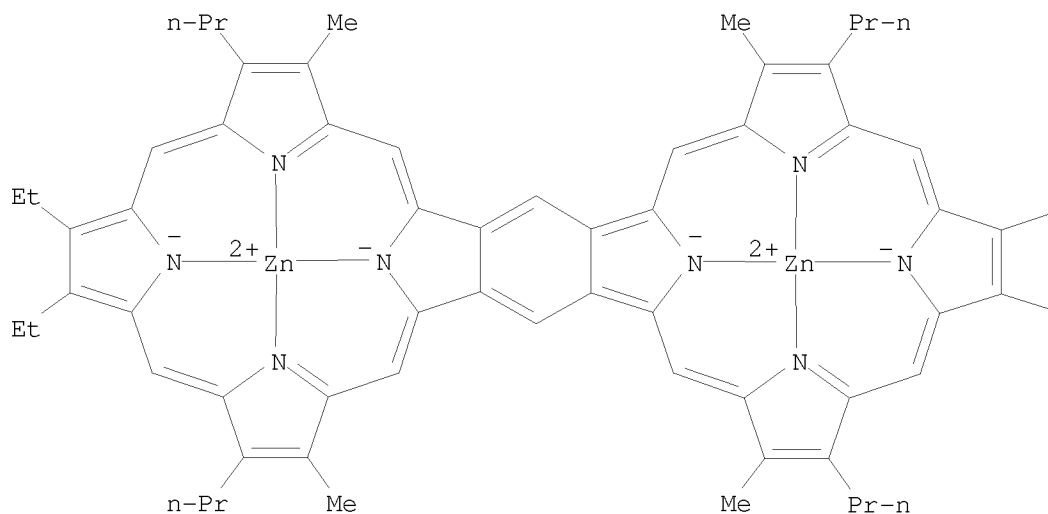
CN 29H,31H-Tetrabenzo[b,g,l,q]porphine (CA INDEX NAME)



RN 910923-74-9 CAPLUS

CN Zinc, [ $\mu$ -[9,10,28,29-tetraethyl-4,15,23,34-tetramethyl-5,14,24,33-tetrapropyl-39H,41H,43H,45H-benzo[1,2-b:4,5-b']diporphinato(4-)- $\kappa$ N39, $\kappa$ N40, $\kappa$ N41, $\kappa$ N42: $\kappa$ N43, $\kappa$ N44, $\kappa$ N45, $\kappa$ N46]]di- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B

Et

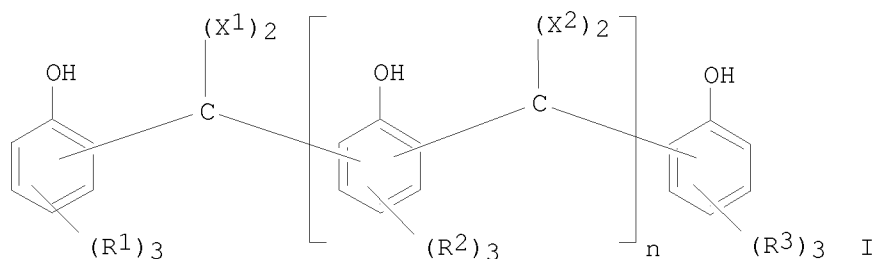
Et

REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

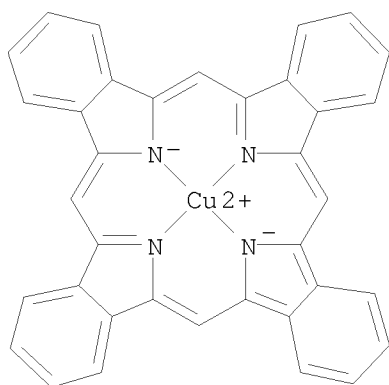
L5 ANSWER 15 OF 26 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2005:1334762 CAPLUS  
 DOCUMENT NUMBER: 144:79408  
 TITLE: Field effect transistor and production process thereof  
 INVENTOR(S): Nakayama, Tomonari; Ohnishi, Toshinobu; Kubota, Makoto  
 PATENT ASSIGNEE(S): Canon Kabushiki Kaisha, Japan  
 SOURCE: PCT Int. Appl., 44 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005122279	A1	20051222	WO 2005-JP10995	20050609
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
JP 2005354012	A	20051222	JP 2004-176130	20040614
US 20070096079	A1	20070503	US 2005-559799	20051208
PRIORITY APPLN. INFO.:			JP 2004-176130	A 20040614
			WO 2005-JP10995	W 20050609

GI

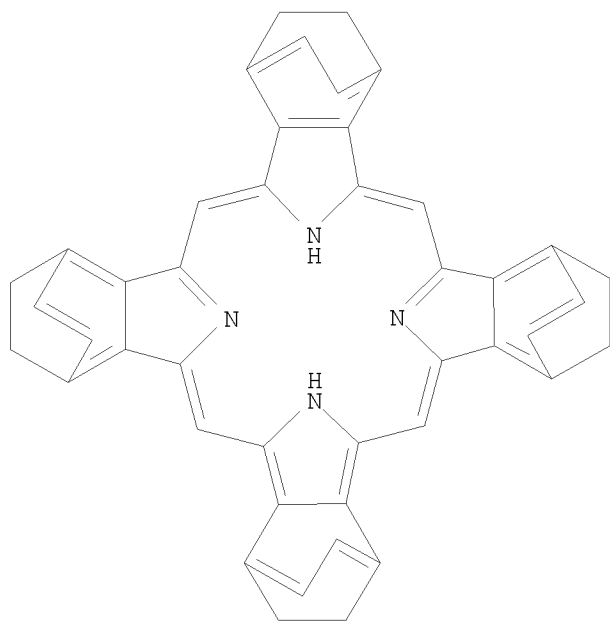


- AB Title field effect transistor includes a substrate, an organic semiconductor layer, an insulating layer, and conductive layers, wherein the insulating layer comprises a cured product of a phenol resin represented by the following general formula (I): (R1, R2 and R3 each represent hydrogen atom, halogen atom, hydroxymethyl group, alkyl group having 1 to 12 carbon atoms, alkenyl group, alkynyl group, alkoxyl group, alkylthio group, or alkyl ester group, X1 and X2 each represent hydrogen atom, alkyl group having 1 to 12 carbon atoms, alkenyl group, alkynyl group, or aryl group, and n represents an integer of 0 to 2,000). According to the present invention, a field effect transistor capable of smoothening the gate electrode having a low surface smoothness, in which a current leak to the gate electrode is small can be obtained.
- IT 21519-18-6, Copper tetrabenzoporphine  
 RL: DEV (Device component use); USES (Uses)  
 (semiconducting layer-containing; production of field effect transistor containing phenolic resin insulating layer)
- RN 21519-18-6 CAPLUS
- CN Copper, [29H,31H-tetrabenzob[b,g,l,q]porphinato(2-)-κN29,κN30,κN31,κN32]-, (SP-4-1)- (CA INDEX NAME)



REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 16 OF 26 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2005:1187544 CAPLUS  
 DOCUMENT NUMBER: 144:43821  
 TITLE: Methanofullerene-coated tetrabenzoporphyrin organic field-effect transistors  
 AUTHOR(S): Shea, Patrick B.; Kanicki, Jerzy; Cao, Yong; Ono, Noboru  
 CORPORATE SOURCE: Organic and Molecular Electronics Laboratory, Department of Electrical Engineering and Computer Science, The University of Michigan, Ann Arbor, MI, 48109, USA  
 SOURCE: Applied Physics Letters (2005), 87(17), 173506/1-173506/3  
 CODEN: APPLAB; ISSN: 0003-6951  
 PUBLISHER: American Institute of Physics  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Organic field-effect transistors (OFETs) using a solution-processable form of the organic semiconductor tetrabenzoporphyrin were fabricated with a top coating of a soluble n-type organic semiconductor. The top coating was found to extend the lifetime of the device in that the field-effect mobility, subthreshold slope, and OFF-state current were maintained at or near their as-fabricated states. O doping by extended air exposure was effectively slowed by the electron-accepting coating layer. Coated devices also display a transfer characteristic indicative of a parasitic latch-up transistor formed at the back channel of the OFETs.  
 IT 201739-37-9  
 RL: PRP (Properties)  
 (CP; methanofullerene-coated tetrabenzoporphyrin organic field-effect transistors)  
 RN 201739-37-9 CAPLUS  
 CN 1,4:8,11:15,18:22,25-Tetraethano-29H,31H-tetrabenzob[b,g,l,q]porphine (9CI)  
 (CA INDEX NAME)



REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 17 OF 26 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:682827 CAPLUS

DOCUMENT NUMBER: 143:397071

TITLE: Electrical properties of staggered electrode, solution-processed, polycrystalline tetrabenzoporphyrin field-effect transistors

AUTHOR(S): Shea, Patrick B.; Johnson, Aaron R.; Ono, Noboru; Kanicki, Jerzy

CORPORATE SOURCE: Department of Electrical Engineering and Computer Science, The University of Michigan, Ann Arbor, MI, 48109, USA

SOURCE: IEEE Transactions on Electron Devices (2005), 52(7), 1497-1503

CODEN: IETDAI; ISSN: 0018-9383

PUBLISHER: Institute of Electrical and Electronics Engineers

DOCUMENT TYPE: Journal

LANGUAGE: English

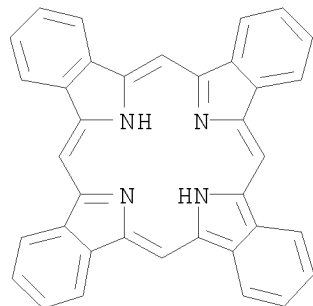
AB We characterize and analyze the elec. performance of solution-processed, polycryst. tetrabenzoporphyrin thin-film field-effect transistors with staggered source and drain contacts. Devices demonstrated a saturation field-effect mobility and threshold voltage on the order of  $10^{-2}$  cm<sup>2</sup>/V-s and -15 V, resp., as well as a subthreshold slope of 1.2 V/decade and an ON-/OFF-current ratio exceeding 105. The device performance and electronic properties of the thin film were used to construct device energy band diagrams. Lastly, the device conduction mechanism is discussed.

IT 52952-31-5, Tetrabenzoporphyrin

RL: DEV (Device component use); USES (Uses)

(elec. properties of staggered electrode, solution-processed, polycryst.

tetrabenzoporphyrin field-effect transistor)  
 RN 52952-31-5 CAPLUS  
 CN 29H,31H-Tetrabenzo[b,g,l,q]porphine (CA INDEX NAME)



REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

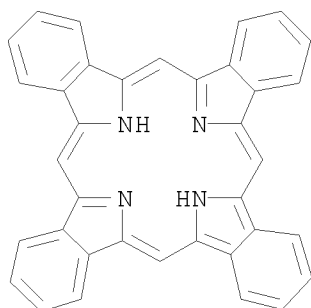
L5 ANSWER 18 OF 26 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2005:655874 CAPLUS  
 DOCUMENT NUMBER: 143:316290  
 TITLE: Field-effect mobility of polycrystalline  
 tetrabenzoporphyrin thin-film transistors  
 AUTHOR(S): Shea, Patrick B.; Kanicki, Jerzy; Ono, Noboru  
 CORPORATE SOURCE: Organic and Molecular Electronics Laboratory,  
 Department of Electrical Engineering and Computer  
 Science, The University of Michigan, Ann Arbor, MI,  
 48109, USA  
 SOURCE: Journal of Applied Physics (2005), 98(1),  
 014503/1-014503/7  
 CODEN: JAPIAU; ISSN: 0021-8979  
 PUBLISHER: American Institute of Physics  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB A possible relation between a thin-film microstructure and an organic  
 thin-film field-effect transistor (OFET) behavior is discussed  
 in terms of nonlinearity in the extraction of the device elec. parameters.  
 Staggered source and drain electrode OFETs were fabricated using a soluble  
 precursor form of the organic small mol. semiconductor tetrabenzoporphyrin,  
 and characterized using linear and nonlinear best-fit methods. Linear  
 best-fit models overestimated the field-effect mobility and accumulation  
 threshold voltage when compared to a nonlinear best-fit model that  
 accounts for dispersive charge-carrier transport. The deviation between  
 the methods is consistently less than that for polymer OFETs, as indicated  
 by smaller nonlinearity factors of  $\gamma$  1.2° and 1.7 in the  
 linear and saturation regimes, resp. The nonlinear field-effect mobility  
 exhibits a sublinear gate-bias dependence wherein the mobility increases  
 at a slower rate in strong accumulation than near threshold. Also,  
 nonlinear curve fitting indicates lower trap characteristic temps. as  
 compared to polymer OFETs, and a relatively moderate d. of grain-boundary  
 trap states localized at the dielec. interface and in the bulk to be  
 filled before accumulation-related conduction dominates.  
 IT 52952-31-5, Tetrabenzoporphyrin  
 RL: PRP (Properties); TEM (Technical or engineered material use); USES

(Uses)

(field-effect mobility of polycryst. tetrabenzoporphyrin thin-film transistors)

RN 52952-31-5 CAPLUS

CN 29H,31H-Tetrabenzo[b,g,l,q]porphine (CA INDEX NAME)



REFERENCE COUNT: 48 THERE ARE 48 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 19 OF 26 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:302391 CAPLUS

DOCUMENT NUMBER: 142:383799

TITLE: Method for evaluation of organic semiconductor materials by measuring optical absorption and manufacture of devices using evaluated materials

INVENTOR(S): Aramaki, Shinji; Kato, Junichi

PATENT ASSIGNEE(S): Mitsubishi Chemical Corp., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 8 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
-----	----	-----	-----	-----
JP 2005091231	A	20050407	JP 2003-326760	20030918
JP 4100310	B2	20080611		

PRIORITY APPLN. INFO.: JP 2003-326760 20030918

AB The method includes preparing plural samples having different carrier mobility, measuring the carrier mobility and optical absorption of the samples, establishing correlation between the measured mobility and purity calculated by the measured optical absorption, measuring optical absorption of target semiconductor materials, and evaluating carrier mobility by comparing purity calculated by the measured optical absorption with the preestablished correlation. Preferably, the organic semiconductor materials have porphyrins and are useful for transistors. Carrier mobility show good correlation with purity calculated by optical absorption.

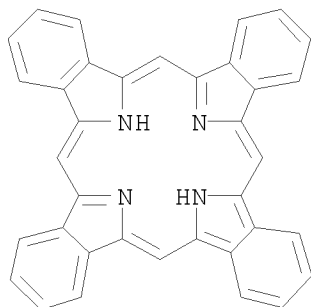
IT 52952-31-5P, 29H,31H-Tetrabenzo[b,g,l,q]porphine

RL: DEV (Device component use); IMF (Industrial manufacture); PREP (Preparation); USES (Uses)

(evaluation of organic semiconductor materials by measuring optical absorption for manufacture of semiconductor devices)



RN 52952-31-5 CAPLUS  
 CN 29H,31H-Tetrabenzo[b,g,l,q]porphine (CA INDEX NAME)



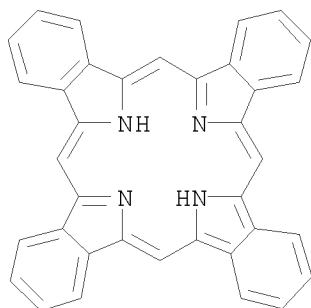
L5 ANSWER 20 OF 26 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2005:238200 CAPLUS  
 DOCUMENT NUMBER: 142:307999  
 TITLE: Organic field-effect transistors  
 INVENTOR(S): Aramaki, Shinji; Tsurutani, Yasuyuki; Sakai, Yoshitada  
 PATENT ASSIGNEE(S): Mitsubishi Chemical Corp., Japan  
 SOURCE: Jpn. Kokai Tokkyo Koho, 14 pp.  
 CODEN: JKXXAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2005072569	A	20050317	JP 2004-224313	20040730
PRIORITY APPLN. INFO.:			JP 2003-287666	A 20030806

AB The gate insulator films of organic FETs are laminates of polymer-containing high-dielec.-constant insulator films and polymer-containing low-dielec.-constant insulator films, where the difference in the dielec. constant of the both insulator films is  $\geq 1$ .

IT 52952-31-5, Tetrabenzoporphyrin  
 RL: DEV (Device component use); USES (Uses)  
 (dielec. constant of gate insulator films of organic FETs)

RN 52952-31-5 CAPLUS  
 CN 29H,31H-Tetrabenzo[b,g,l,q]porphine (CA INDEX NAME)



L5 ANSWER 21 OF 26 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2005:217013 CAPLUS  
 DOCUMENT NUMBER: 142:307926  
 TITLE: Design and fabrication of a field effect transistor with an organic semiconductor layer of tetrabenzocopper porphyrin  
 INVENTOR(S): Miura, Daisuke; Nakayama, Tomonari; Ohnishi, Toshinobu; Kubota, Makoto  
 PATENT ASSIGNEE(S): Canon Kabushiki Kaisha, Japan  
 SOURCE: PCT Int. Appl., 36 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005022649	A1	20050310	WO 2004-JP12044	20040817
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
JP 2005079204	A	20050324	JP 2003-305487	20030828
US 20060145141	A1	20060706	US 2005-545398	20050812
US 7285441	B2	20071023		
US 20080048185	A1	20080228	US 2007-892326	20070822
US 7394096	B2	20080701		
PRIORITY APPLN. INFO.:			JP 2003-305487	A 20030828
			WO 2004-JP12044	W 20040817
			US 2005-545398	A3 20050812
OTHER SOURCE(S): MARPAT 142:307926				
AB The present invention relates to a field effect transistor having an organic semiconductor layer using a tetrabenzocopper porphyrin crystal and to a method for manufacturing the field effect transistor.				

The field effect transistor has an organic semiconductor layer, which contains at least one tetrabenzocopper porphyrin crystal and has peaks at  $\geq 2$  of Bragg angles ( $2\theta$ ) in  $\text{CuK}\alpha$  x-ray diffraction of  $8.4^\circ \pm 0.2^\circ$ ,  $10.2^\circ \pm 0.2^\circ$ ,  $11.8^\circ \pm 0.2^\circ$ , and  $16.9^\circ \pm 0.2^\circ$ .

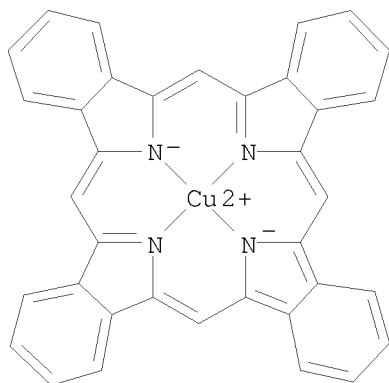
IT 21519-18-6

RL: DEV (Device component use); USES (Uses)

(design and fabrication of a field effect transistor with an organic semiconductor layer of tetrabenzocopper porphyrin)

RN 21519-18-6 CAPLUS

CN Copper, [29H,31H-tetrabenzocopper(II)porphyrinato(2-)- $\kappa\text{N}29,\kappa\text{N}30,\kappa\text{N}31,\kappa\text{N}32$ ]-, (SP-4-1)- (CA INDEX NAME)



REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 22 OF 26 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:986131 CAPLUS

DOCUMENT NUMBER: 141:430596

TITLE: Manufacture of high-purity porphyrins for field-effect transistors

INVENTOR(S): Aramaki, Shinji; Kato, Junichi

PATENT ASSIGNEE(S): Mitsubishi Chemical Corp., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 17 pp.

CODEN: JKXXAF

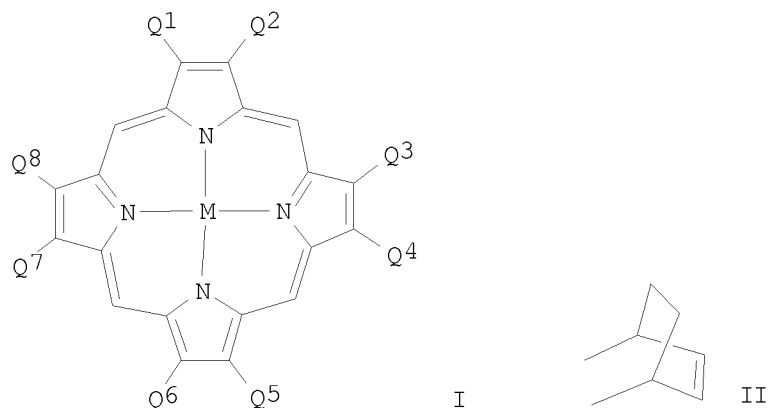
DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
-----	----	-----	-----	-----
JP 2004323376	A	20041118	JP 2003-116711	20030422
PRIORITY APPLN. INFO.:			JP 2003-116711	20030422
OTHER SOURCE(S):	MARPAT	141:430596		
GI				

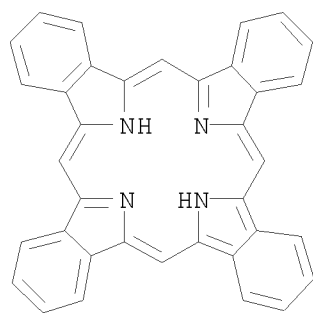


AB The porphyrins I (Z1-Z8 = monovalent organic group;  $\geq 1$  of Q1Q2, Q3Q4, Q5Q6, and Q7Q8 form II; M = two H, metal) are manufactured by oxidation of porphyrinogens, where the content of aldehydes other than HCHO or their precursor alcs. is  $\leq 20$  mol or  $\leq 80$  mol to 1 mol porphyrinogens, resp. before and/or during the oxidation. Thus, Et 4,7-dihydro-4,7-ethano-2H-isoindole-1-carboxylate was reduced, treated with p-MeC6H4SO3H, and oxidized with chloranil to give I (Q1Q2, Q3Q4, Q5Q6, and Q7Q8 form II; M = two H), which was spin-coated between source and drain electrodes, and heated to give a field-effect transistor showing high saturation mobility.

IT 52952-31-5P, 29H,31H-Tetrabenzo[b,g,l,q]porphine  
 RL: DEV (Device component use); PNU (Preparation, unclassified); PREP (Preparation); USES (Uses)  
 (manufacture of high-purity porphyrins for field-effect transistors by oxidation of porphyrinogens under control of aldehyde and alc. content)

RN 52952-31-5 CAPLUS

CN 29H,31H-Tetrabenzo[b,g,l,q]porphine (CA INDEX NAME)



L5 ANSWER 23 OF 26 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2004:857665 CAPLUS  
 DOCUMENT NUMBER: 141:359266  
 TITLE: Field effect transistor and method of producing the same  
 INVENTOR(S): Miura, Daisuke; Nakayama, Tomonari

PATENT ASSIGNEE(S): Canon Kabushiki Kaisha, Japan  
 SOURCE: PCT Int. Appl., 37 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004087836	A1	20041014	WO 2004-JP4346	20040326
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
JP 2004320007	A	20041111	JP 2004-106680	20040331
US 20060099732	A1	20060511	US 2005-535202	20050517
US 7094625	B2	20060822		
PRIORITY APPLN. INFO.:			JP 2003-96210	A 20030331
			WO 2004-JP4346	W 20040326

OTHER SOURCE(S): MARPAT 141:359266

AB A field effect transistor having a high field effect mobility is provided which can be obtained by a simple method. The field effect transistor includes an organic semiconductor layer composed of a crystallized film of a naphthoporphyrin compound, which is obtained by the conversion by heating of the coating film of a porphyrin compound, the organic semiconductor layer having crystal grains with a maximum diameter of 1 mm or more.

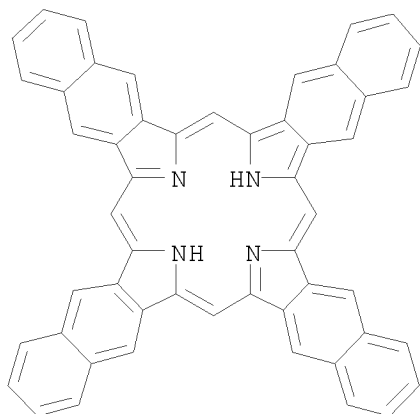
IT 73523-25-8P 776295-35-3P

RL: DEV (Device component use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)

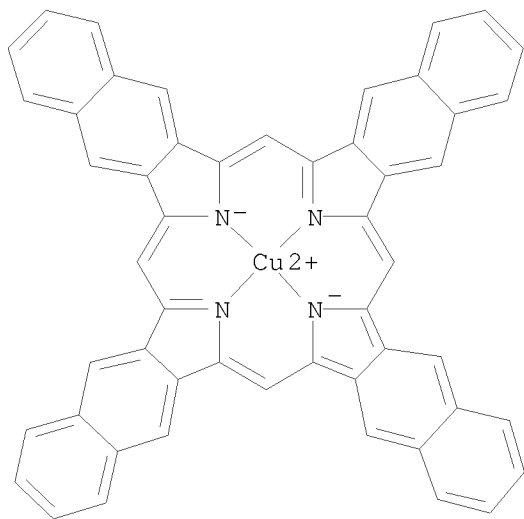
(films, active layer; method of producing field effect transistor including crystallized naphthoporphyrin compound, obtained by conversion of coating film of porphyrin compound)

RN 73523-25-8 CAPLUS

CN 37H,39H-Tetranaphtho[2,3-b:2',3'-g:2'',3'''-l:2''',3'''-q]porphine (CA INDEX NAME)



RN 776295-35-3 CAPLUS  
 CN Copper, [37H,39H-tetranaphtho[2,3-b:2',3'-g:2'',3''-l:2''',3'''-q]porphinato(2-)-κN37,κN38,κN39,κN40]-, (SP-4-1)-  
 (9CI) (CA INDEX NAME)

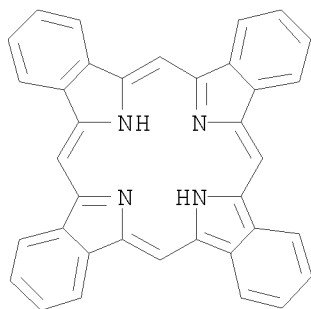


REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 24 OF 26 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2004:652219 CAPLUS  
 DOCUMENT NUMBER: 141:183119  
 TITLE: Field-effect transistors  
 INVENTOR(S): Aramaki, Shinji  
 PATENT ASSIGNEE(S): Mitsubishi Chemical Corp., Japan  
 SOURCE: Jpn. Kokai Tokkyo Koho, 18 pp.  
 CODEN: JKXXAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	JP 2004228371	A	20040812	JP 2003-15057	20030123
PRIORITY APPLN. INFO.:				JP 2003-15057	20030123
AB	FETs contain organic semiconductor films which have different d. distribution of oxidation- or reduction-type elec. conductivity yielders in regions constituting source and/or drain electrodes. The FETs have smooth carrier flow from the source and/or drain electrodes into semiconductor layers.				
IT	52952-31-5, Tetrabenzoporphyrin RL: DEV (Device component use); USES (Uses) (FETs containing organic semiconductor films)				
RN	52952-31-5 CAPLUS				
CN	29H,31H-Tetrabenzob[b,g,l,q]porphine (CA INDEX NAME)				

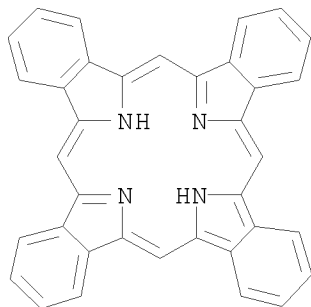


L5 ANSWER 25 OF 26 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2004:236771 CAPLUS  
 DOCUMENT NUMBER: 140:432116  
 TITLE: Solution-processible organic semiconductor for transistor applications: Tetrabenzoporphyrin  
 AUTHOR(S): Aramaki, Shinji; Sakai, Yoshimasa; Ono, Noboru  
 CORPORATE SOURCE: Mitsubishi Chemical Group Science and Technology Research Center, Inc., Aoba-ku, Yokohama, 227-8502, Japan  
 SOURCE: Applied Physics Letters (2004), 84(12), 2085-2087  
 CODEN: APPLAB; ISSN: 0003-6951  
 PUBLISHER: American Institute of Physics  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB The authors report an organic semiconductor, tetrabenzoporphyrin, that can be used for transistor applications. It can be derived from a soluble precursor compound with bicyclo structure. The precursor film is amorphous and shows good film morphol. Then it is converted into an insol. crystalline semiconductor film quant. at elevated temperature of 150-200°. Field-effect transistors were fabricated by this method. Observed mobility of the devices exceeded 10-2 cm2/V s with appropriate process and device structure.  
 IT 52952-31-5P, Tetrabenzoporphyrin  
 RL: PNU (Preparation, unclassified); PRP (Properties); TEM (Technical or

engineered material use); PREP (Preparation); USES (Uses)  
(tetrabenzoporphyrin as solution-processible organic semiconductor for  
transistor applications)

RN 52952-31-5 CAPLUS

CN 29H,31H-Tetrabenzo[b,g,l,q]porphine (CA INDEX NAME)



REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 26 OF 26 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2003:766184 CAPLUS

DOCUMENT NUMBER: 140:68049

TITLE: 29H,31H-Tetrabenzo[b,g,l,q]porphin

AUTHOR(S): Aramaki, Shinji; Mizuguchi, Jin

CORPORATE SOURCE: Mitsubishi Chemical Corporation, Science and  
Technology Research Center Inc., Aoba-ku, Yokohama,  
227-8502, Japan

SOURCE: Acta Crystallographica, Section E: Structure Reports  
Online (2003), E59(10), o1556-o1558  
CODEN: ACSEBH; ISSN: 1600-5368  
URL: <http://journals.iucr.org/e/issues/2003/10/00/ob6299/index.html>

PUBLISHER: International Union of Crystallography

DOCUMENT TYPE: Journal; (online computer file)

LANGUAGE: English

AB The title compound, C<sub>36</sub>H<sub>22</sub>N<sub>4</sub>, has recently been found to exhibit an  
excellent field effect transistor characteristic. The mol. is  
not entirely flat in its crystal structure (i.e. not D<sub>2h</sub>) but is slightly  
deformed, as characterized by crystallog. Ci symmetry. The mols. are  
stacked along the b axis in a herring-bone fashion. Crystallog. data are  
given.

IT 52952-31-5, 29H,31H-Tetrabenzo[b,g,l,q]porphine

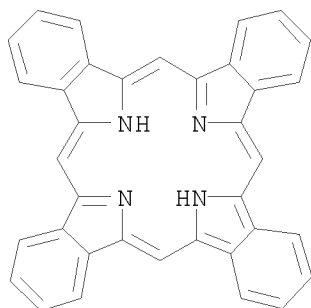
RL: PRP (Properties)

(crystal structure of)

RN 52952-31-5 CAPLUS

CN 29H,31H-Tetrabenzo[b,g,l,q]porphine (CA INDEX NAME)





REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> log h

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION

FULL ESTIMATED COST

144.78	323.35
--------	--------

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION

CA SUBSCRIBER PRICE

-20.80	-20.80
--------	--------

SESSION WILL BE HELD FOR 120 MINUTES

STN INTERNATIONAL SESSION SUSPENDED AT 10:39:08 ON 19 DEC 2008

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSPTAJRK1626

PASSWORD:

\* \* \* \* \* RECONNECTED TO STN INTERNATIONAL \* \* \* \* \*

SESSION RESUMED IN FILE 'CAPLUS' AT 11:00:19 ON 19 DEC 2008

FILE 'CAPLUS' ENTERED AT 11:00:19 ON 19 DEC 2008

COPYRIGHT (C) 2008 AMERICAN CHEMICAL SOCIETY (ACS)

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION

FULL ESTIMATED COST

144.78	323.35
--------	--------

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION

CA SUBSCRIBER PRICE

-20.80	-20.80
--------	--------

=> d his

(FILE 'HOME' ENTERED AT 10:37:11 ON 19 DEC 2008)

10583126.trn

FILE 'REGISTRY' ENTERED AT 10:37:23 ON 19 DEC 2008

L1 STRUCTURE UPLOADED  
L2 50 L1  
L3 1509 L1 FULL

FILE 'CAPLUS' ENTERED AT 10:37:53 ON 19 DEC 2008

L4 948 L3  
L5 26 L4 AND TRANSISTOR

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	144.78	323.35
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-20.80	-20.80

FILE 'REGISTRY' ENTERED AT 11:00:31 ON 19 DEC 2008

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

COPYRIGHT (C) 2008 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 17 DEC 2008 HIGHEST RN 1086212-50-1

DICTIONARY FILE UPDATES: 17 DEC 2008 HIGHEST RN 1086212-50-1

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH July 5, 2008.

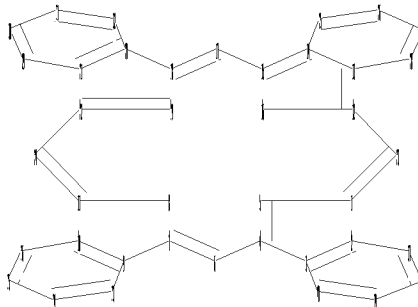
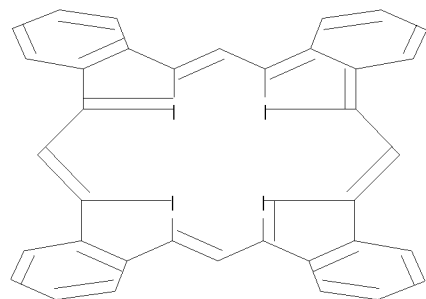
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10583126\Struc 2.str



10583126.trn

```

ring nodes :
1  2  3  4  5  6  7  8  9 10 11 12 13 14 15 16 17 18 19 20 21 22 23
24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40
ring bonds :
1-2 1-5 1-23 2-3 2-37 3-4 3-40 4-5 4-6 6-7 7-8 7-9 8-11 9-10 9-33
10-11 10-36 11-24 12-13 12-16 12-23 13-14 13-28 14-15 14-25 15-16 15-17
17-18 18-19 18-20 19-22 20-21 20-32 21-22 21-29 22-24 25-26 26-27 27-28
29-30 30-31 31-32 33-34 34-35 35-36 37-38 38-39 39-40
exact/norm bonds :
7-8 8-11 12-16 15-16
normalized bonds :
1-2 1-5 1-23 2-3 2-37 3-4 3-40 4-5 4-6 6-7 7-9 9-10 9-33 10-11 10-36
11-24 12-13 12-23 13-14 13-28 14-15 14-25 15-17 17-18 18-19 18-20 19-22
20-21 20-32 21-22 21-29 22-24 25-26 26-27 27-28 29-30 30-31 31-32 33-34
34-35 35-36 37-38 38-39 39-40

```

```

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom
29:Atom 30:Atom 31:Atom 32:Atom 33:Atom 34:Atom 35:Atom 36:Atom 37:Atom
38:Atom 39:Atom 40:Atom

```

L6           STRUCTURE UPLOADED

=> l1 not l6

SAMPLE SEARCH INITIATED 11:00:57 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED -       799 TO ITERATE

100.0% PROCESSED       799 ITERATIONS                   14 ANSWERS  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:   ONLINE   \*\*COMPLETE\*\*  
                          BATCH    \*\*COMPLETE\*\*  
PROJECTED ITERATIONS:       14285 TO   17675  
PROJECTED ANSWERS:         56 TO       504

L7           14 SEA SSS SAM L1 NOT L6

=> l1 not l6 full

FULL SEARCH INITIATED 11:01:01 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED -   15629 TO ITERATE

100.0% PROCESSED       15629 ITERATIONS               363 ANSWERS  
SEARCH TIME: 00.00.01

L8           363 SEA SSS FUL L1 NOT L6

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	178.36	501.71

10583126.trn

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-20.80

FILE 'CAPLUS' ENTERED AT 11:01:04 ON 19 DEC 2008  
 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
 PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
 COPYRIGHT (C) 2008 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 19 Dec 2008 VOL 149 ISS 26  
 FILE LAST UPDATED: 18 Dec 2008 (20081218/ED)

Caplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2008.

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

<http://www.cas.org/legal/infopolicy.html>

=> l8

L9 103 L8

=> d ibib abs hitstr 1-103

L9 ANSWER 1 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2008:1056455 CAPLUS

DOCUMENT NUMBER: 149:434800

TITLE: Complicated Fermi-type vibronic resonance: Untangling of the single-site quasi-line fluorescence excitation spectra of a methylated dibenzoporphin

AUTHOR(S): Arabei, S. M.; Kuzmitsky, V. A.; Solovyov, K. N.

CORPORATE SOURCE: Stepanov Institute of Physics, NAS of Belarus B.I., Minsk, 220072, Belarus

SOURCE: Chemical Physics (2008), 352(1-3), 197-204

CODEN: CMPHC2; ISSN: 0301-0104

PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The quasi-line low-temperature (4.2 K) fluorescence excitation spectra of 2,3,12,13-tetramethyldibenzo[g,q]porphin introduced into an n-octane matrix were measured in the range of the S<sub>2</sub> ← S<sub>0</sub> electronic transition at selective fluorescence monitoring for the 2 main types of impurity centers (sites). A characteristic feature of these spectra is that a conglomerate of quasi-lines - a structured complex band - is observed

instead of one 0-0 quasi-line of the  $S_2 \leftarrow S_0$  transition. In this band, the intensity distributions for the 2 main sites considerably differ from each other. The occurrence of such conglomerates is interpreted as a result of nonadiabatic vibrational-electronic interaction between the vibronic  $S_2$  and  $S_1$  states (the complex vibronic analog of the Fermi resonance). The frequencies and intensities of individual transitions determined from the deconvolution of complex conglomerates are used as the initial data for solving the inverse spectroscopic problem: the determination

of

the unperturbed electronic and vibrational levels of states involved in the resonance and the vibronic-interaction matrix elements between them. This problem is solved with a method developed previously. The exptl. results and their anal. are compared to the analogous data obtained earlier for meso-tetraazaporphin and meso-tetrapropylporphin. The energy intervals between the  $S_2$  and  $S_1$  electronic levels ( $\Delta E_{S_2S_1}$ ) of the 2 main types of impurity centers formed by mols. of a given porphyrin in the crystal matrix significantly differ from each other, the values of this difference ( $\delta \Delta E_{S_2S_1}$ ) being considerably greater for tetramethyldibenzoporphin,  $\delta \Delta E_{S_2S_1} = 228 \text{ cm}^{-1}$ , than for the 2 other porphyrins. At the same time, the energies of the unperturbed vibrational states of the  $S_1$  electronic level participating in the resonance are very close to each other for these 2 sites.

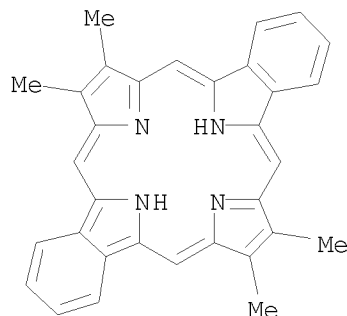
IT 157869-32-4

RL: PRP (Properties)

(untangling of single-site quasi-line fluorescence excitation spectra of methylated dibenzoporphin with complicated Fermi-type vibronic resonance)

RN 157869-32-4 CAPLUS

CN 25H,27H-Dibenzo[b,l]porphine, 8,9,20,21-tetramethyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 2 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2008:856762 CAPLUS

DOCUMENT NUMBER: 149:189210

TITLE: Novel organic precursor compound and method of producing organic semiconductor device

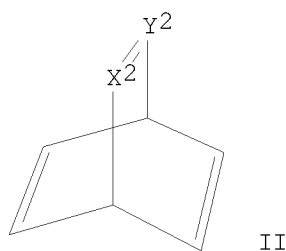
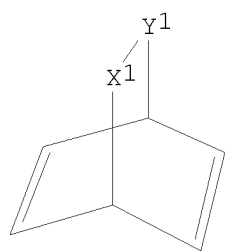
INVENTOR(S): Masumoto, Akane; Kikuchi, Toshihiro; Ono, Noboru; Uno, Hidemitsu; Nakashima, Hiroko

PATENT ASSIGNEE(S): Canon Kabushiki Kaisha, Japan; Ehime University

SOURCE: U.S. Pat. Appl. Publ., 58pp.

CODEN: USXXCO  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20080171403	A1	20080717	US 2007-964619	20071226
PRIORITY APPLN. INFO.:			JP 2006-352555	A 20061227
			JP 2007-232091	A 20070906
OTHER SOURCE(S):	MARPAT 149:189210			
GI				



AB A method of producing an organic semiconductor device is provided in which a layer composed of an organic semiconductor having excellent crystallinity and orientation in a low-temperature region can be formed, and the device can be produced in the air. The method includes forming a layer composed of an organic semiconductor precursor on a base body and irradiating the organic semiconductor precursor with light, wherein the organic semiconductor precursor is a porphyrin compound or an azaporphyrin compound having in its mol. at least one of the structure represented by the following general formula (I) where X1 and Y1 each independently represent O, S, carbonyl, thiocarbonyl, CR1R2 or NR3, and R1-R3 are each H, linear or branched C1-12 alkyl, alkenyl, alkoxy, alkylthio, alkyl ester, or aryl groups, or hydroxyl but X1 and Y1 are not CR1R2 at the same time. Alternatively, the structure has formula (II) where X2=Y2 is N-N or CR4=N and R4 is H, a C1-12 linear or branched alkyl, alkenyl, alkoxy, alkylthio, alkyl ester, or aryl group, or hydroxyl. The precursor porphyrin or azaporphyrin may contain a coupled ring structure formed by this structure. In addition to the organic semiconductor layer, a crystallization promoting layer, preferably

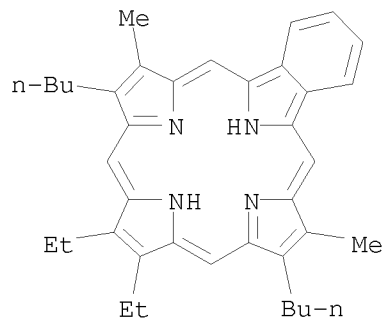
a polysiloxane compound, may be provided. The precursor compds. and method are particularly suited for fabrication of thin film transistors.

IT 1039105-62-8P  
 RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(target precursor; organic precursor compound and method of producing organic semiconductor device)

RN 1039105-62-8 CAPLUS

CN 23H,25H-Benzo[b]porphine, 9,18-dibutyl-13,14-diethyl-8,19-dimethyl- (CA INDEX NAME)



L9 ANSWER 3 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2008:492936 CAPLUS

DOCUMENT NUMBER: 149:93859

TITLE: Chemical transformations of mono- and bis(buta-1,3-dien-1-yl)porphyrins: a new synthetic approach to mono- and dibenzoporphyrins

AUTHOR(S): Silva, Ana M. G.; de Oliveira, Kleber T.; Faustino, Maria A. F.; Neves, Maria G. P. M. S.; Tome, Augusto C.; Silva, Artur M. S.; Cavaleiro, Jose A. S.; Brandao, Paula; Felix, Vitor

CORPORATE SOURCE: Department of Chemistry, University of Aveiro, Aveiro, 3810-193, Port.

SOURCE: European Journal of Organic Chemistry (2008), (4), 704-712

CODEN: EJOCFK; ISSN: 1434-193X

PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 149:93859

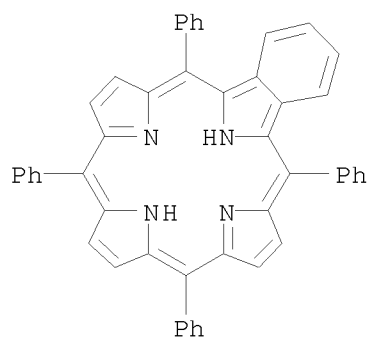
AB  $\beta$ -Butadienyl- and  $\beta,\beta'$ -dibutadienylporphyrins were prepared by the Wittig reaction of  $\beta$ -formyl- and  $\beta,\beta'$ -diformyl-meso-tetraphenylporphyrins with allylic P ylide. Subsequent treatment of  $\beta$ -butadienylporphyrin with dienophiles afforded the corresponding Diels-Alder adducts. In the absence of dienophiles,  $\beta$ -butadienylporphyrin underwent electrocyclization, followed by oxidation, to give monobenzoporphyrin in good yield. Similarly, adjacent and opposite dibenzoporphyrins were successfully synthesized from adjacent and opposite  $\beta,\beta'$ -dibutadienylporphyrins, resp. This is the 1st report of electrocyclization of  $\beta$ -butadienylporphyrins. The structures of mono- and dibenzoporphyrin Ni complexes, and of a Diels-Alder adduct, were determined by single-crystal x-ray diffraction; a strong distortion from the planarity of the porphyrin core was observed

IT 915093-05-9 915093-06-0 1033305-44-0

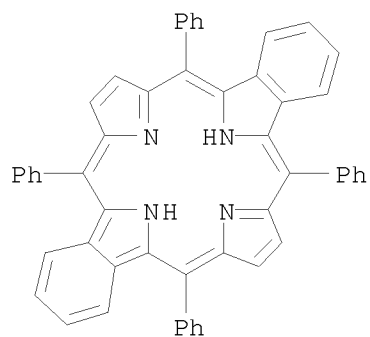
RL: FMU (Formation, unclassified); FORM (Formation, nonpreparative) (formation and UV-visible spectrum of)

RN 915093-05-9 CAPLUS

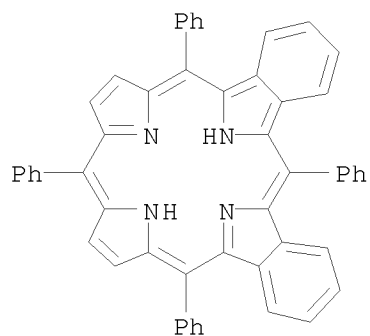
CN 23H,25H-Benzo[b]porphine, 6,11,16,21-tetraphenyl- (9CI) (CA INDEX NAME)



RN 915093-06-0 CAPLUS  
 CN 25H,27H-Dibenzo[b,l]porphine, 6,11,18,23-tetraphenyl- (9CI) (CA INDEX NAME)



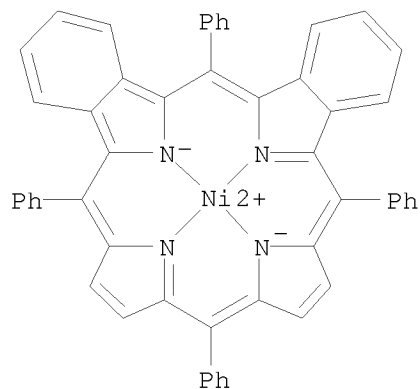
RN 1033305-44-0 CAPLUS  
 CN 25H,27H-Dibenzo[b,g]porphine, 6,11,16,23-tetraphenyl- (CA INDEX NAME)



IT 1033305-29-1P 1033305-31-5P  
 RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation, crystal structure and demetalation of)  
 RN 1033305-29-1 CAPLUS

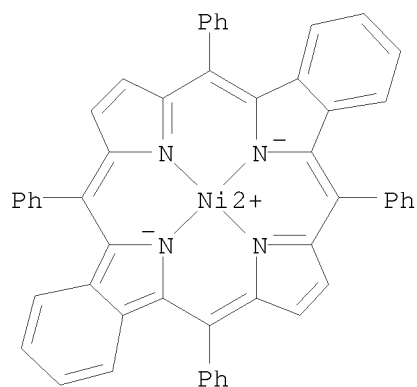


CN Nickel, [6,11,16,23-tetraphenyl-25H,27H-dibenzo[b,g]porphinato(2-)-  
κN25,κN26,κN27,κN28]-, (SP-4-2)- (CA INDEX NAME)



RN 1033305-31-5 CAPLUS

CN Nickel, [6,11,18,23-tetraphenyl-25H,27H-dibenzo[b,l]porphinato(2-)-  
κN25,κN26,κN27,κN28]-, (SP-4-1)- (CA INDEX NAME)



IT 1033305-27-9P

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP  
(Preparation); RACT (Reactant or reagent)

(preparation, crystal structure, demetalation and reaction with dienophiles)

RN 1033305-27-9 CAPLUS

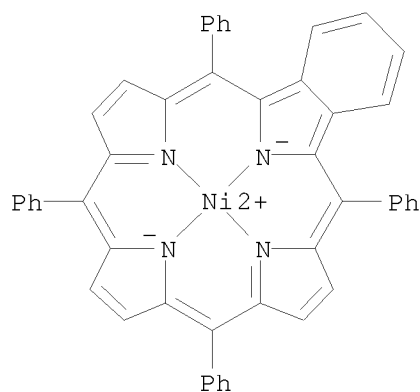
CN Nickel, [6,11,16,21-tetraphenyl-23H,25H-benzo[b]porphinato(2-)-  
κN23,κN24,κN25,κN26]-, (SP-4-2)-, compd. with  
trichloromethane (1:1) (CA INDEX NAME)

CM 1

CRN 1033305-26-8

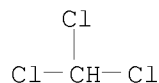
CMF C48 H30 N4 Ni

CCI CCS



CM 2

CRN 67-66-3  
CMF C H Cl3



REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 4 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2008:490559 CAPLUS

DOCUMENT NUMBER: 149:53762

TITLE: Thermal behavior of free-base and core-modified bicyclo[2.2.2]octadiene-fused porphyrins

AUTHOR(S): Uno, Hidemitsu; Shimizu, Yusuke; Uoyama, Hiroki; Tanaka, Yousuke; Okujima, Tetsuo; Ono, Noboru

CORPORATE SOURCE: Division of Synthesis and Analysis, Department of Molecular Science, Integrated Center for Sciences (INCS), Ehime University and CREST, Japan Science and Technology Agency (JST), Matsuyama, 790-8577, Japan

SOURCE: European Journal of Organic Chemistry (2008), (1), 87-98

CODEN: EJOCFK; ISSN: 1434-193X

PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Multistep thermal fragmentation of quadruply bicyclo[2.2.2]-octadiene-fused porphyrins giving tetrabenzoporphyrins was examined in detail. After the first extrusion of an ethylene mol. from the porphyrin derivative, the opposite bicyclo-[2.2.2]octadiene moiety preferentially underwent the second retro-Diels-Alder reaction to give an opp-dibenzoporphyrin derivative rather than an adj-dibenzoporphyrin derivative. These two benzoporphyrin derivs. then decomposed to give a tribenzoporphyrin derivative in similar rates. The temperature regions of these fragmentations could

not be distinguished by thermogravimetric anal. In contrast, the third and the fourth fragmentations obviously occurred stepwise. There was a temperature region where the tribenzoporphyrin derivative preferentially existed.

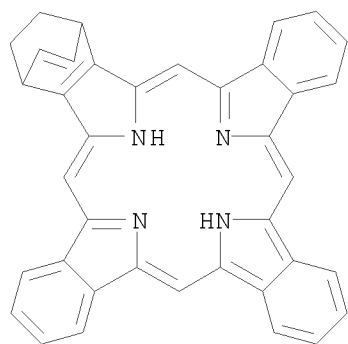
In the case of the 21,23-dithiaporphyrin derivative, opp-21,23-dithiadibenzoporphyrin, possessing benzo moieties fused at the pyrrole parts of the core-modified porphyrin chromophore was predominantly formed during the fragmentation. In the case of the 21-thiaporphyrin derivative, an ethylene mol. was extruded selectively from the bicyclo[2.2.2]octadiene moiety adjacent to the thiophene part to give 21-thiabenzo[q]porphyrin and then 21-thiabenzo[g,q]porphyrin derivs. In these cases, the last ethylene extrusion also occurred very slowly.

IT 1032406-95-3P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(crystal structure; thermal fragmentation/retro-Diels-Alder reaction of  
free-base and core-modified bicyclo[2.2.2]octadiene-fused porphyrins)

RN 1032406-95-3 CAPLUS

CN 1,4-Ethano-29H,31H-tetrabenzo[b,g,l,q]porphine, 1,4-dihydro- (CA INDEX  
NAME)



REFERENCE COUNT: 57 THERE ARE 57 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 5 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2007:1075858 CAPLUS

DOCUMENT NUMBER: 147:552996

TITLE: Novel preparation of fluorinated isoindoles and their  
conversion to fluorinated benzoporphyrins

AUTHOR(S): Uno, Hidemitsu; Masuda, Go; Tukiiji, Marie; Nishioka,  
Yuiko; Iida, Toshiya

CORPORATE SOURCE: Division of Synthesis and Analysis, Department of  
Molecular Science, Integrated Center for Sciences,  
Japan Science Technology Agency (JST), Ehime  
University and CREST, Matsuyama, 790-8577, Japan

SOURCE: Tetrahedron Letters (2007), 48(42), 7512-7515

CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: Elsevier Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 147:552996

AB 4,5,6,7-Tetrafluoroisoindole and their related compds. were prepared  
directly from the corresponding phthalonitriles by reduction with a hydride

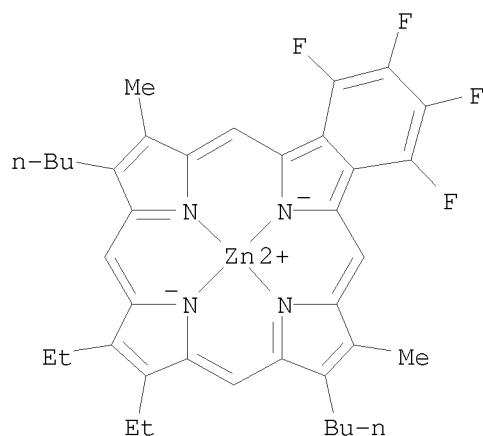
reagent such as DIBAL or catalytic hydrogenation in the presence of an acid. 4,5,6,7-Tetrafluoroisoindole was converted to fluorinated benzoporphyrins and zincated derivative

IT 957468-01-8P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of fluorinated benzoporphyrin from tetrafluoroisoindole)

RN 957468-01-8 CAPLUS

CN Zinc, [9,18-dibutyl-13,14-diethyl-1,2,3,4-tetrafluoro-8,19-dimethyl-23H,25H-benzo[b]porphinato(2-)-κN23,κN24,κN25,κN26]-, (SP-4-1)- (CA INDEX NAME)



REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 6 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2007:909991 CAPLUS

DOCUMENT NUMBER: 149:448084

TITLE: Synthesis and spectral properties of unsymmetrical benzoporphyrins containing phenoxy groups or quinoxaline fragments

AUTHOR(S): Galanin, N. E.; Shaposhnikov, G. P.

CORPORATE SOURCE: Ivanovo State University of Chemical Technology, Ivanovo, 153000, Russia

SOURCE: Russian Journal of Organic Chemistry (2007), 43(7), 1080-1086

CODEN: RJOCEQ; ISSN: 1070-4280

PUBLISHER: Pleiades Publishing, Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Condensation of phthalimide and 4-tert-butylphthalimide with zinc(II) acetate gave 3-(3-oxo-2,3-dihydro-1H-isoindol-1-ylidenemethyl)-1H-isoindol-1-one and 5-tert-butyl-3-(5-tert-butyl-3-oxo-2,3-dihydro-1H-isoindol-1-ylidenemethyl)-1H-isoindol-1-one, resp. Their reactions with 4-phenoxyphthalimide and quinoxaline-2,3-dicarboximide in the presence of Zn(OAc)<sub>2</sub> gave zinc complexes of cis-4,4'-diphenoxytetrabenzoporphyrin and cis-di(4-tert-butylbenzo)diquinoxalinoporphyrin. The complexes were converted into the free bases by treatment with sulfuric acid. Spectral properties of the obtained porphyrin derivs. were studied.

IT 1070317-63-3P

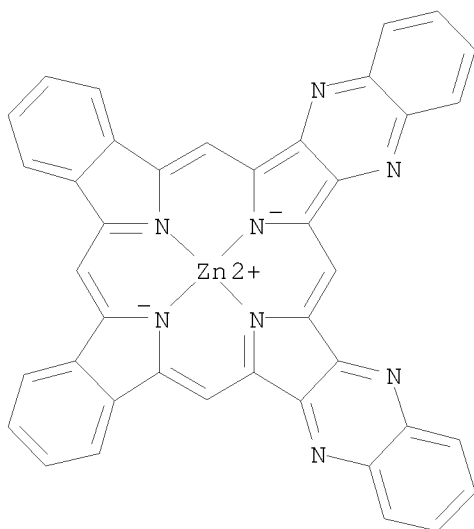
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)

(preparation and demetalation of unsym. zinc benzoporphyrins)

RN 1070317-63-3 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

PAGE 1-A



PAGE 2-A

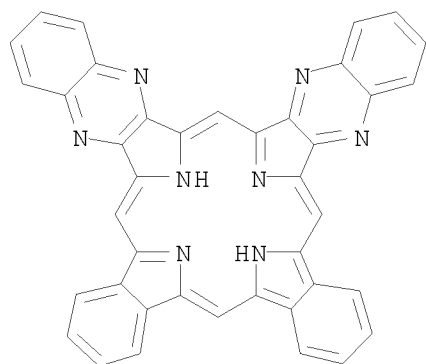
2 ( D1-Bu-t )

IT 1070317-66-6P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of unsym. benzoporphyrins)

RN 1070317-66-6 CAPLUS

CN INDEX NAME NOT YET ASSIGNED



2 ( D1-Bu-t )

REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 7 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2007:802775 CAPLUS

DOCUMENT NUMBER: 147:355485

TITLE: Synthesis of porphyrin dimers fused with a benzene unit

AUTHOR(S): Uno, Hidemitsu; Nakamoto, Ken-ichi; Kuroki, Kenji; Fujimoto, Akiko; Ono, Noboru

CORPORATE SOURCE: Division of Synthesis and Analysis, Department of Molecular Science Integrated Center for Sciences (INCS), Ehime University, Matsuyama, 790-8577, Japan

SOURCE: Chemistry--A European Journal (2007), 13(20), 5773-5784

CODEN: CEUJED; ISSN: 0947-6539

PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 147:355485

AB Bicyclo[2.2.2]octadiene-connected pyrrolo-porphyrins were prepared by an inverse-type [3 + 1] porphyrin synthesis of a bicyclo[2.2.2]octadiene-fused dipyrrole with a tripyrrane dicarbaldehyde. Another [3 + 1] porphyrin synthesis of pyrrole-connected porphyrins with the same or other tripyrrane dicarbaldehydes gave bicyclo[2.2.2]octadiene-bridged diporphyrins, the central metals and/or peripheral substituents of which were different. Thermal decomposition of the bicyclo[2.2.2]octadiene skeleton to a benzene moiety gave  $\pi$ -system-fused porphyrin dimers in a highly pure form.

IT 949012-73-1P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and crystal structure of)

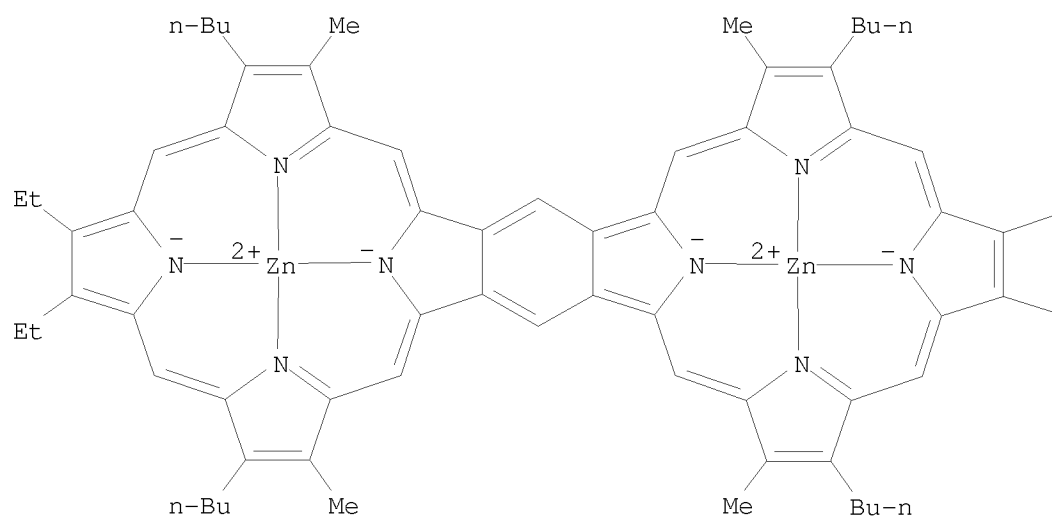
RN 949012-73-1 CAPLUS

CN Zinc, [ $\mu$ -[5,14,24,33-tetraethyl-9,10,28,29-tetraethyl-4,15,23,34-tetramethyl-39H,41H,43H,45H-benzo[1,2-b:4,5-b']diporphinato(4-)- $\kappa$ N39, $\kappa$ N40, $\kappa$ N41, $\kappa$ N42: $\kappa$ N43, $\kappa$ N44, $\kappa$ N45, $\kappa$ N46]]di-, compd. with pyridine (1:4) (CA INDEX NAME)

CM 1

CRN 406483-35-0  
 CMF C70 H78 N8 Zn2  
 CCI CCS

PAGE 1-A



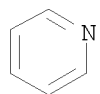
PAGE 1-B

Et

Et

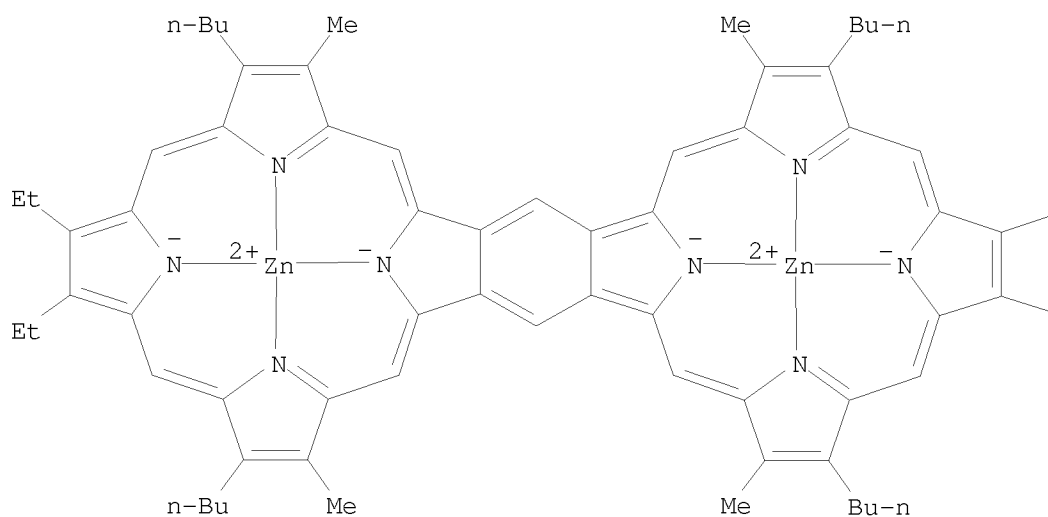
CM 2

CRN 110-86-1  
 CMF C5 H5 N



IT 406483-35-0P 949012-59-3P 949012-61-7P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (preparation of)  
 RN 406483-35-0 CAPLUS  
 CN Zinc, [ $\mu$ -[5,14,24,33-tetrabutyl-9,10,28,29-tetraethyl-4,15,23,34-  
 tetramethyl-39H,41H,43H,45H-benzo[1,2-b:4,5-b']diporphinato(4-)-  
 $\kappa$ N39, $\kappa$ N40, $\kappa$ N41, $\kappa$ N42: $\kappa$ N43, $\kappa$ N44, $\kappa$ N  
 45, $\kappa$ N46]]di- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B

Et

Et

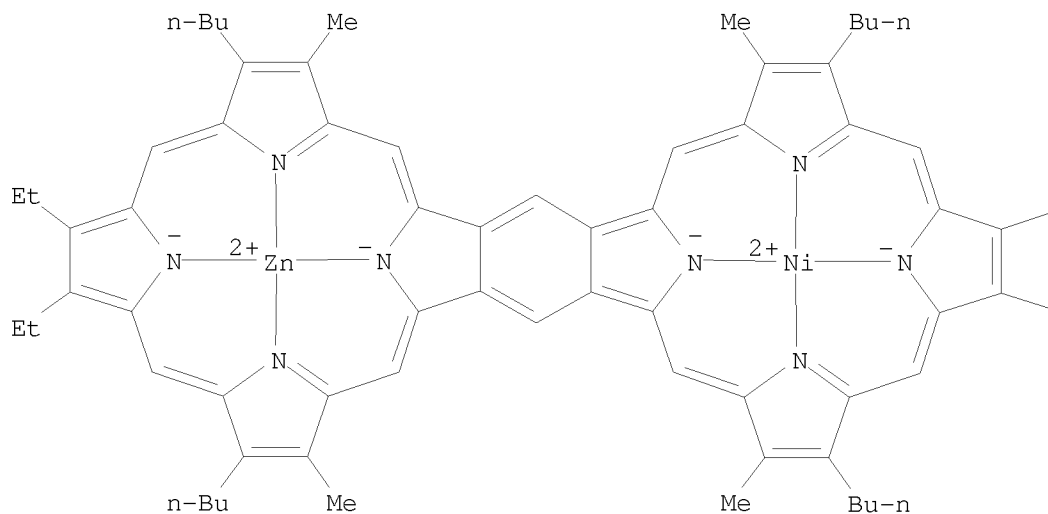
RN 949012-59-3 CAPLUS

10583126.trn



CN Nickel, [ $\mu$ -[5,14,24,33-tetrabutyl-9,10,28,29-tetraethyl-4,15,23,34-tetramethyl-39H,41H,43H,45H-benzo[1,2-b:4,5-b']diporphinato(4-)- $\kappa$ N39, $\kappa$ N40, $\kappa$ N41, $\kappa$ N42: $\kappa$ N43, $\kappa$ N44, $\kappa$ N45, $\kappa$ N46]](zinc)- (CA INDEX NAME)

PAGE 1-A

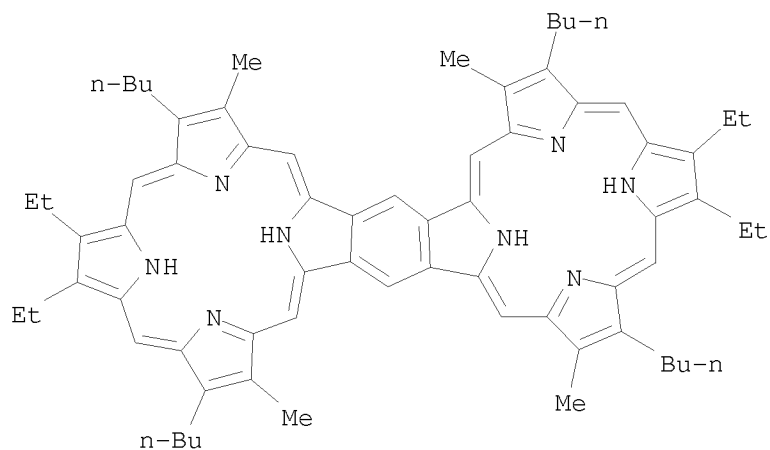


PAGE 1-B

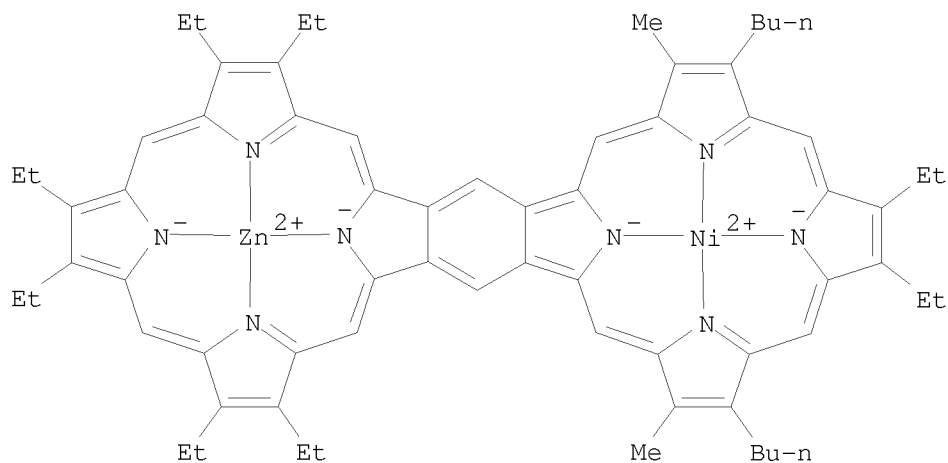
Et

Et

RN 949012-61-7 CAPLUS  
CN 39H,41H,43H,45H-Benzo[1,2-b:4,5-b']diporphine,  
5,14,24,33-tetrabutyl-9,10,28,29-tetraethyl-4,15,23,34-tetramethyl- (CA  
INDEX NAME)



IT 949012-69-5P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 RN 949012-69-5 CAPLUS  
 CN Nickel, [ $\mu$ -[[5,14-dibutyl-9,10,23,24,28,29,33,34-octaethyl-4,15-dimethyl-39H,41H,43H,45H-benzo[1,2-b:4,5-b']diporphinato(4-)- $\kappa$ N39, $\kappa$ N40, $\kappa$ N41, $\kappa$ N42: $\kappa$ N43, $\kappa$ N44, $\kappa$ N45, $\kappa$ N46]]](zinc)- (CA INDEX NAME)



REFERENCE COUNT: 45 THERE ARE 45 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 8 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2007:436957 CAPLUS  
 DOCUMENT NUMBER: 147:300608  
 TITLE: Electronic structures and spectra of porphyrin with fused benzoheterocycles: DFT and TDDFT-PCM investigations  
 AUTHOR(S): Zhu, Yulan; Zhou, Shuyu; Kan, Yuhe; Su, Zhongmin

CORPORATE SOURCE: Department of Chemistry, Jiangsu Province Key  
Laboratory for Chemistry of Low-dimensional Materials,  
Huaiyin Teachers College, Huaiyin, Jiangsu, 223300,  
Peop. Rep. China

SOURCE: International Journal of Quantum Chemistry (2007),  
107(7), 1614-1623  
CODEN: IJQCB2; ISSN: 0020-7608

PUBLISHER: John Wiley & Sons, Inc.

DOCUMENT TYPE: Journal

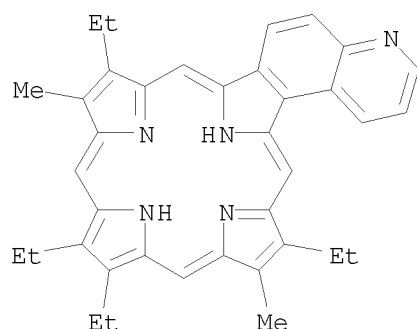
LANGUAGE: English

AB D. functional theory (DFT) and time-dependent DFT (TDDFT) are applied to study seven asym.  $\pi$ -conjugated porphyrins with extended benzoheterocycles: quinoline, indole, benzoimidazole, benzothiazole, benzoxazole, 2,1,3-benzothiadiazole, and 2,1,3-benzoxadiazole. The solvation effects on the excitation energies for these porphyrin derivs. in chloroform are taken into account by using the continuum model (C-PCM) combined with TDDFT, and this method makes a closer agreement with the exptl. values, especially for the B-bands of these objects. Great efforts have been made on investigating the influences of the fused aromatic units of the porphyrins on the absorption properties as these can be particularly important for many applications. Benzoheterocycle introduction and solvent effects have been systemically investigated, and close agreement is obtained between calculated and measured UV-vis spectra. These theor. data could shed light on future synthetic chemical

IT 312273-73-7 947151-93-1 947151-94-2  
947151-95-3 947151-96-4  
RL: PRP (Properties)  
(DFT study on electronic structures and spectra of porphyrin with fused benzoheterocycles)

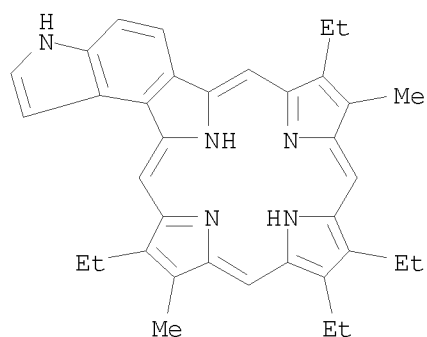
RN 312273-73-7 CAPLUS

CN 25H,27H-Quino[5,6-b]porphine, 10,15,16,21-tetraethyl-11,20-dimethyl- (CA INDEX NAME)

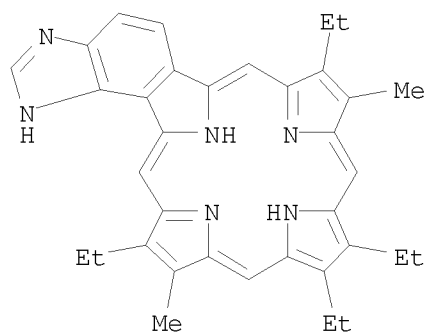


RN 947151-93-1 CAPLUS

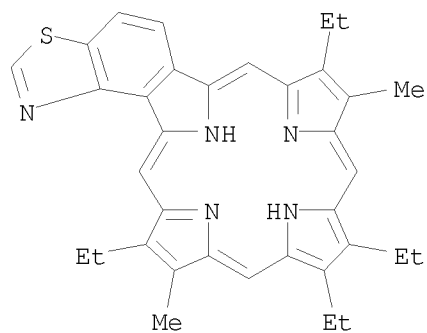
CN 3H,24H,26H-Indolo[4,5-b]porphine, 9,14,15,20-tetraethyl-10,19-dimethyl- (CA INDEX NAME)



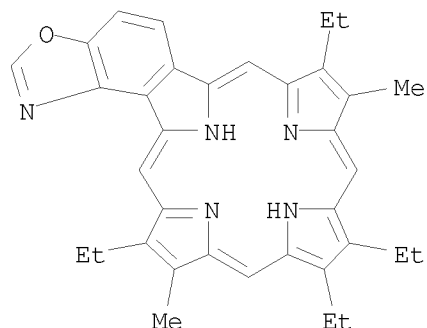
RN 947151-94-2 CAPLUS  
 CN 1H,24H,26H-Benzimidazo[4,5-b]porphine,  
 9,14,15,20-tetraethyl-10,19-dimethyl- (CA INDEX NAME)



RN 947151-95-3 CAPLUS  
 CN 24H,26H-Benzothiazolo[4,5-b]porphine,  
 9,14,15,20-tetraethyl-10,19-dimethyl- (CA INDEX NAME)



RN 947151-96-4 CAPLUS  
 CN 24H,26H-Benzoxazolo[4,5-b]porphine, 9,14,15,20-tetraethyl-10,19-dimethyl-  
 (CA INDEX NAME)



REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 9 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2006:1252123 CAPLUS

DOCUMENT NUMBER: 146:154706

TITLE: C-F Bond Activation by Modified Sulfonatodehalogenation: Facile Synthesis and Properties of Novel Tetrafluorobenzoporphyrins by Direct Intramolecular Cyclization and Reductive Defluorinative Aromatization of Readily Available  $\beta$ -Perfluoroalkylated Porphyrins

AUTHOR(S): Liu, Chao; Shen, Dong-Mei; Zeng, Zhuo; Guo, Can-Cheng; Chen, Qing-Yun

CORPORATE SOURCE: Key Laboratory of Organofluorine Chemistry, Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, Shanghai, 200032, Peop. Rep. China

SOURCE: Journal of Organic Chemistry (2006), 71(26), 9772-9783 CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 146:154706

AB A facile and efficient synthesis of various novel fluorinated extended porphyrins was developed. The method is based on the direct intramol. cyclization and reductive defluorinative aromatization of readily available  $\beta$ -perfluoroalkylated porphyrins by highly selective C-F bond activation under modified sulfonatodehalogenation reaction conditions. Various  $\beta$ -( $\omega$ -chloroperfluoroalkyl)-meso-tetraphenylporphyrins prepared readily by sulfonatodehalogenation reaction or palladium-catalyzed cross-coupling reaction were treated with Na<sub>2</sub>S<sub>2</sub>O<sub>4</sub>/K<sub>2</sub>CO<sub>3</sub> (10:10 equiv per RF tail) in DMSO at 100° for 10-30 min, resulting in good yields of novel  $\beta$ -tetrafluorobenzo-meso-tetraphenylporphyrins. That further reduction of C-F bonds of the products was not observed under the optimal conditions indicates the high selectivity of the reaction. The amount of sodium dithionite, base, and central metal ion of substrate porphyrins play important roles in the reaction. Detailed mechanism investigations and systematic studies on x-ray crystallog. structure and photophys. and electrochem. properties of new tetrafluorobenzoporphyrins are also reported.

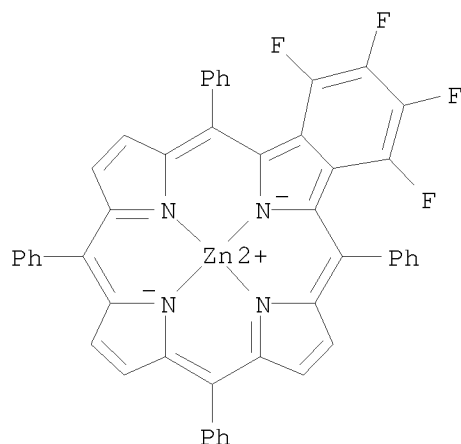
IT 848394-49-0P

RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)

(crystal structure and electrochem. properties of zinc tetrafluorobenzoporphyrin prepared by intramol. cyclization and reductive defluorinative aromatization of perfluoroalkylated porphyrin)

RN 848394-49-0 CAPLUS

CN Zinc, [1,2,3,4-tetrafluoro-6,11,16,21-tetraphenyl-23H,25H-benzo[b]porphinato(2-)-κN23,κN24,κN25,κN26]-, (SP-4-1)- (CA INDEX NAME)



IT 919528-38-4P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(crystal structure of zinc tetrafluorobenzoporphyrin prepared by intramol. cyclization and reductive defluorinative aromatization of perfluoroalkylated porphyrin)

RN 919528-38-4 CAPLUS

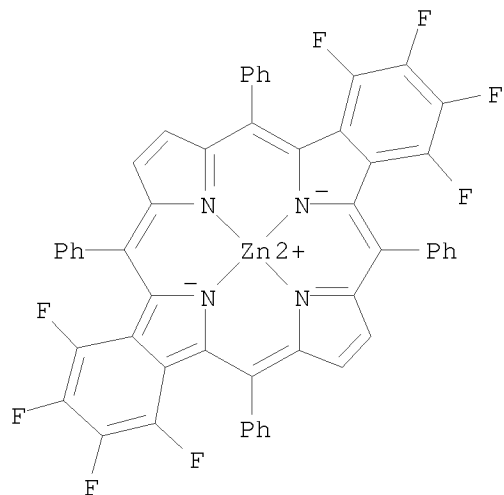
CN Zinc, [1,2,3,4,13,14,15,16-octafluoro-6,11,18,23-tetraphenyl-25H,27H-dibenzo[b,1]porphinato(2-)-κN25,κN26,κN27,κN28]-, (SP-4-1)-, compd. with tetrahydrofuran, hydrate (1:4:1) (CA INDEX NAME)

CM 1

CRN 919528-20-4

CMF C52 H24 F8 N4 Zn

CCI CCS



CM 2

CRN 109-99-9

CMF C4 H8 O



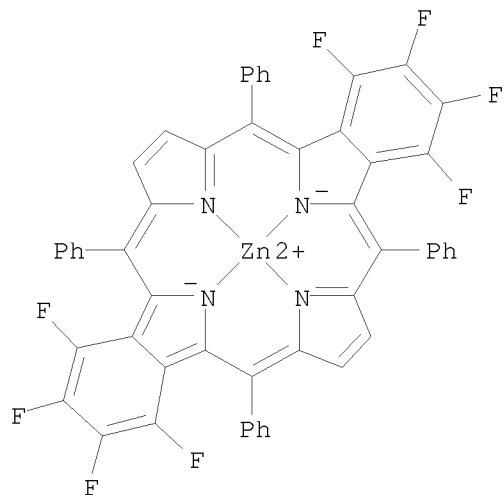
IT 919528-20-4P

RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)

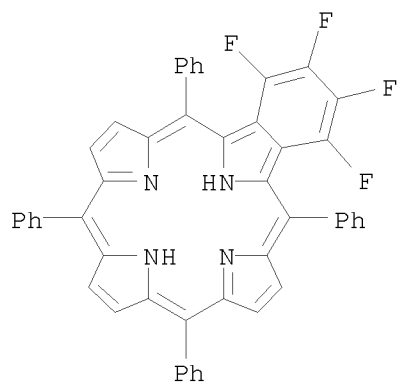
(electrochem. properties of zinc tetrafluorobenzoporphyrin prepared by intramol. cyclization and reductive defluorinative aromatization of perfluoroalkylated porphyrin)

RN 919528-20-4 CAPLUS

CN Zinc, [1,2,3,4,13,14,15,16-octafluoro-6,11,18,23-tetraphenyl-25H,27H-dibenzo[b,1]porphinato(2-)-κN25,κN26,κN27,κN28]-, (SP-4-1)- (CA INDEX NAME)

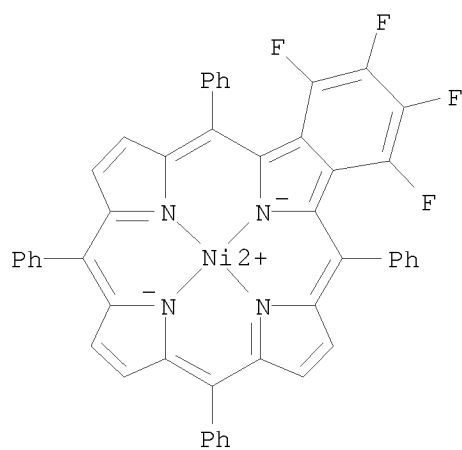


IT 848394-52-5P 919528-14-6P 919528-16-8P  
 919528-19-1P 919528-22-6P 919528-24-8P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of tetrafluorobenzoporphyrins by intramol. cyclization and  
 reductive defluorinative aromatization of perfluoroalkylated  
 porphyrins)  
 RN 848394-52-5 CAPLUS  
 CN 23H,25H-Benzo[b]porphine, 1,2,3,4-tetrafluoro-6,11,16,21-tetraphenyl- (CA  
 INDEX NAME)

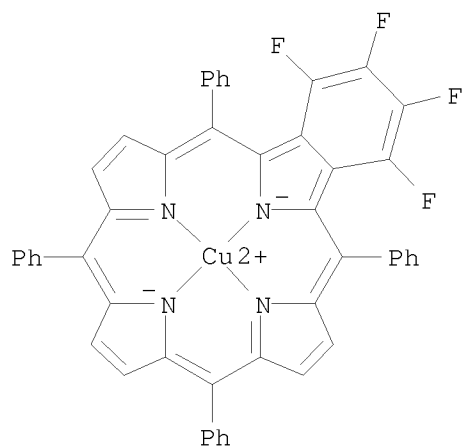


RN 919528-14-6 CAPLUS  
 CN Nickel, [1,2,3,4-tetrafluoro-6,11,16,21-tetraphenyl-23H,25H-  
 benzo[b]porphinato(2-)-κN23,κN24,κN25,κN26]-,  
 (SP-4-1)- (CA INDEX NAME)

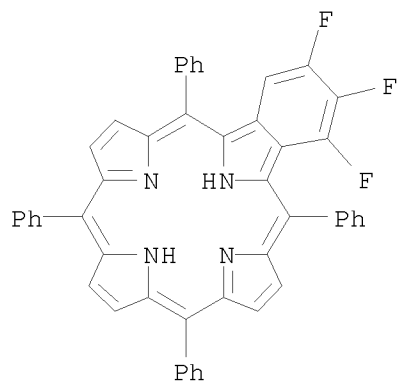




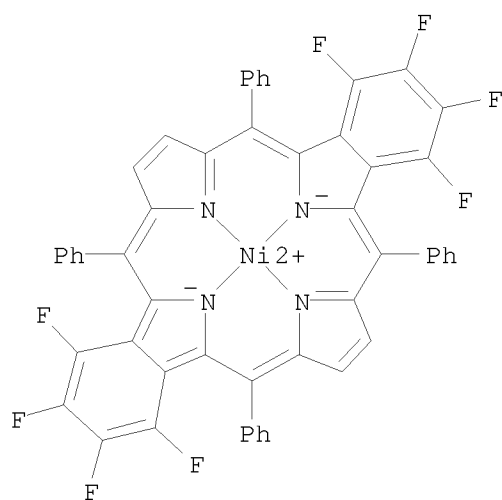
RN 919528-16-8 CAPLUS  
 CN Copper, [1,2,3,4-tetrafluoro-6,11,16,21-tetraphenyl-23H,25H-benzo[b]porphinato(2-)-κN23,κN24,κN25,κN26]-, (SP-4-1)- (CA INDEX NAME)



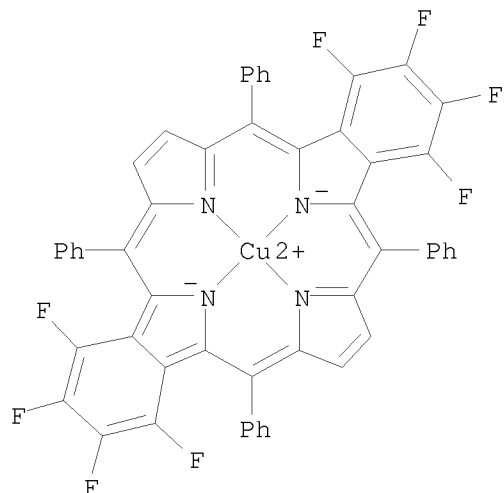
RN 919528-19-1 CAPLUS  
 CN 23H,25H-Benzo[b]porphine, 1,2,3-trifluoro-6,11,16,21-tetraphenyl- (CA INDEX NAME)



RN 919528-22-6 CAPLUS  
 CN Nickel, [1,2,3,4,13,14,15,16-octafluoro-6,11,18,23-tetraphenyl-25H,27H-dibenzo[b,1]porphinato(2-)-κN25,κN26,κN27,κN28]-, (SP-4-1)- (CA INDEX NAME)



RN 919528-24-8 CAPLUS  
 CN Copper, [1,2,3,4,13,14,15,16-octafluoro-6,11,18,23-tetraphenyl-25H,27H-dibenzo[b,1]porphinato(2-)-κN25,κN26,κN27,κN28]-, (SP-4-1)- (CA INDEX NAME)



REFERENCE COUNT: 95 THERE ARE 95 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 10 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2006:1110757 CAPLUS

DOCUMENT NUMBER: 146:81693

TITLE: The first example of Diels-Alder cycloaddition of ortho-xylylenes to meso-tetraarylporphyrins containing electron-deficient  $\beta,\beta$ -double bonds

AUTHOR(S): Ostrowski, Stanislaw; Wyrebek, Przemyslaw

CORPORATE SOURCE: Institute of Chemistry, University of Podlasie, Siedlce, 08-110, Pol.

SOURCE: Tetrahedron Letters (2006), 47(47), 8437-8440

CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: Elsevier Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 146:81693

AB  $\beta$ -Nitro-5,10,15,20-tetraphenylporphyrin and its zinc complex, or 2,7-dinitro-5,10,15,20-tetraphenylporphyrin, react with 1,3-dihydrobenzo[c]thiophene 2,2-dioxide in refluxing 1,2,4-trichlorobenzene, giving rise to chlorins, bacteriochlorins or isobacteriochlorins. The products obtained are attractive intermediates for further functionalization of porphyrins and may be of potential use as sensitizers in photodynamic therapy.

IT 193283-52-2P 916993-50-5P 916993-51-6P

916993-54-9P 916993-55-0P 917392-92-8P

917392-95-1P

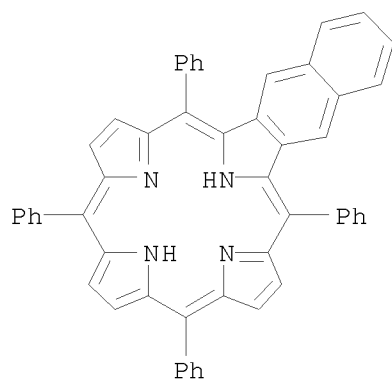
RL: SPN (Synthetic preparation); PREP (Preparation)

(Diels-Alder cycloaddn. of ortho-xylylene to

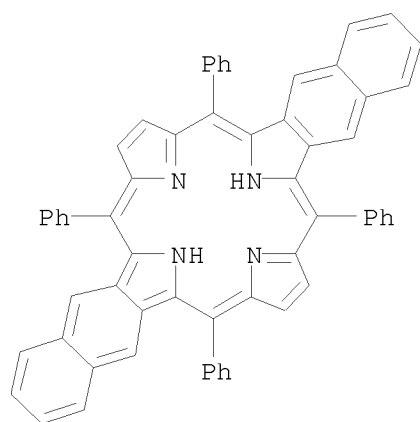
meso-tetraphenylporphyrins)

RN 193283-52-2 CAPLUS

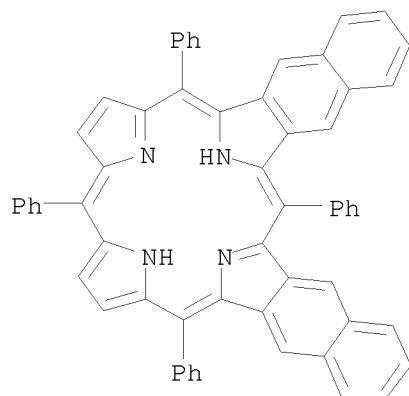
CN 25H,27H-Naphtho[2,3-b]porphine, 7,12,17,22-tetraphenyl- (CA INDEX NAME)



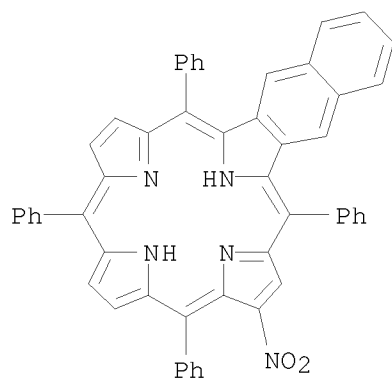
RN 916993-50-5 CAPLUS  
 CN 29H,31H-Dinaphtho[2,3-b:2',3'-l]porphine, 7,12,21,26-tetraphenyl- (CA  
 INDEX NAME)



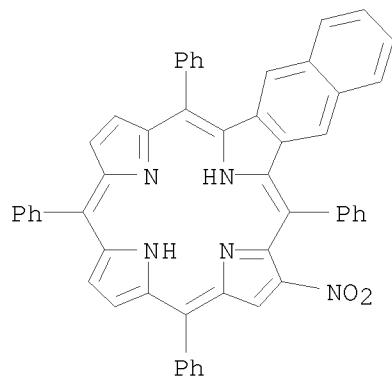
RN 916993-51-6 CAPLUS  
 CN 29H,31H-Dinaphtho[2,3-b:2',3'-g]porphine, 7,12,17,26-tetraphenyl- (CA  
 INDEX NAME)



RN 916993-54-9 CAPLUS  
 CN 25H,27H-Naphtho[2,3-b]porphine, 10-nitro-7,12,17,22-tetraphenyl- (CA INDEX NAME)

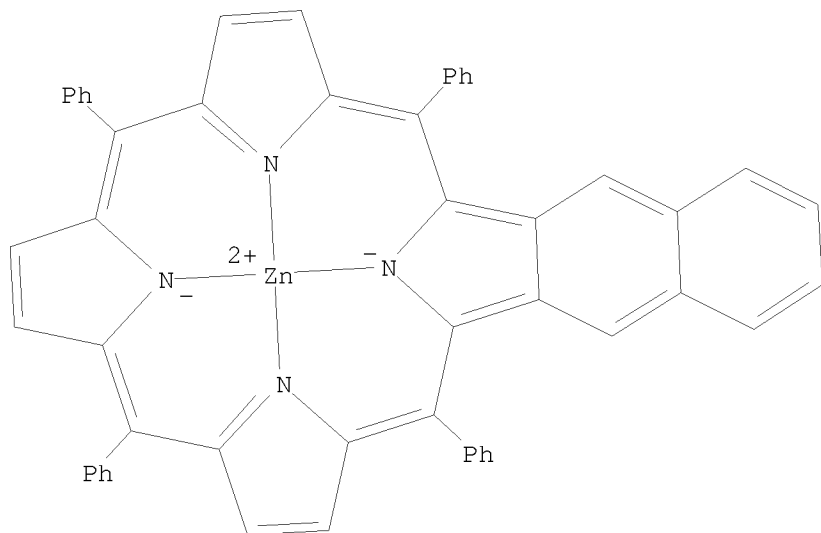


RN 916993-55-0 CAPLUS  
 CN 25H,27H-Naphtho[2,3-b]porphine, 9-nitro-7,12,17,22-tetraphenyl- (CA INDEX NAME)



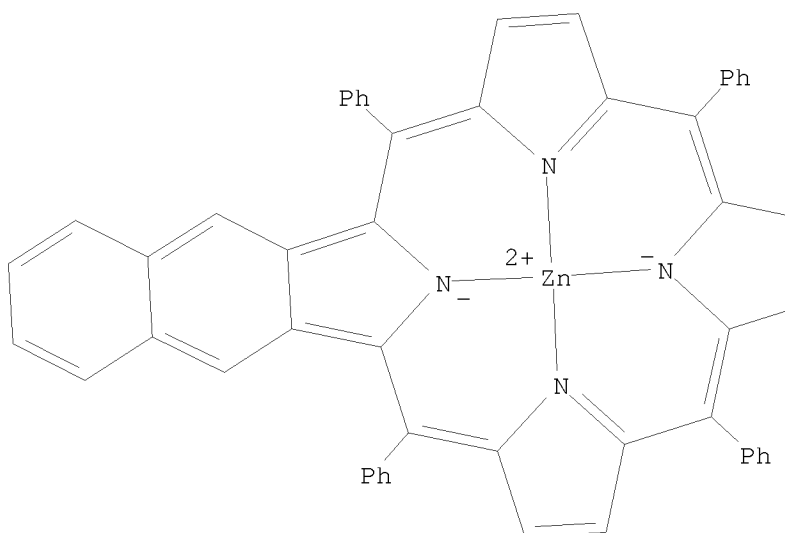
RN 917392-92-8 CAPLUS

CN Zinc, [7,12,17,22-tetraphenyl-25H,27H-naphtho[2,3-b]porphinato(2-)-  
κN25,κN26,κN27,κN28]-, (SP-4-1)- (CA INDEX NAME)

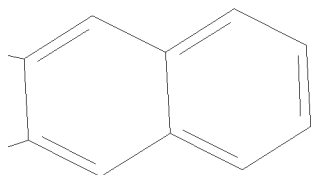


RN 917392-95-1 CAPLUS

CN Zinc, [7,12,21,26-tetraphenyl-29H,31H-dinaphtho[2,3-b:2',3'-1]porphinato(2-)-  
κN29,κN30,κN31,κN32]-, (SP-4-1)- (CA INDEX NAME)

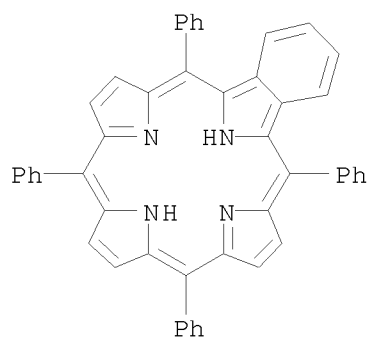


PAGE 1-A

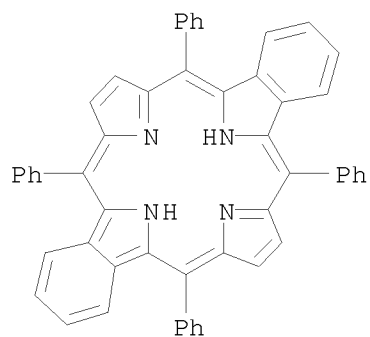


REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

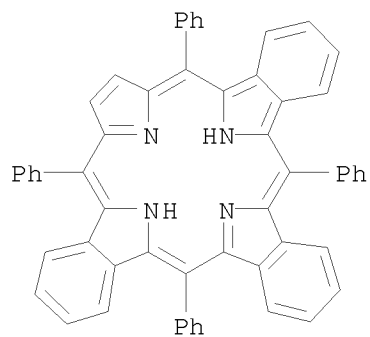
L9 ANSWER 11 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 2006:979857 CAPLUS  
DOCUMENT NUMBER: 145:505241  
TITLE: Benzoporphyrins via an olefin ring-closure metathesis methodology  
AUTHOR(S): Jiao, Lijuan; Hao, Erhong; Fronczek, Frank R.; Vicente, M. Graca H.; Smith, Kevin M.  
CORPORATE SOURCE: Department of Chemistry, Louisiana State University, Baton Rouge, LA, 70803, USA  
SOURCE: Chemical Communications (Cambridge, United Kingdom) (2006), (37), 3900-3902  
CODEN: CHCOFS; ISSN: 1359-7345  
PUBLISHER: Royal Society of Chemistry  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 145:505241  
AB A new route to benzoporphyrins is reported in which readily available vicinal dibromoporphyrins are bis-allylated using the Suzuki reaction, cyclized by way of olefin metathesis and finally oxidized to give mono-, di-, or tri-benzoporphyrins.  
IT 915093-05-9P 915093-06-0P 915093-07-1P  
915093-10-6P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of benzoporphyrins via Suzuki reaction and ring-closing metathesis)  
RN 915093-05-9 CAPLUS  
CN 23H,25H-Benzo[b]porphine, 6,11,16,21-tetraphenyl- (9CI) (CA INDEX NAME)



RN 915093-06-0 CAPLUS  
 CN 25H,27H-Dibenzo[b,l]porphine, 6,11,18,23-tetraphenyl- (9CI) (CA INDEX NAME)

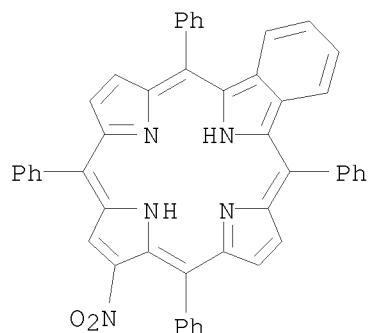


RN 915093-07-1 CAPLUS  
 CN 27H,29H-Tribenzo[b,g,l]porphine, 6,13,20,25-tetraphenyl- (9CI) (CA INDEX NAME)



RN 915093-10-6 CAPLUS  
 CN 23H,25H-Benzo[b]porphine, 2-nitro-5,10,15,20-tetraphenyl- (9CI) (CA INDEX NAME)





REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 12 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2006:93393 CAPLUS

DOCUMENT NUMBER: 144:323611

TITLE: A new synthesis of acenaphthobenzoporphyrin and fluoranthobenzoporphyrin

AUTHOR(S): Okujima, Tetsuo; Komobuchi, Naoki; Uno, Hidemitsu; Ono, Noboru

CORPORATE SOURCE: Department of Chemistry, Faculty of Science, Ehime University, Matsuyama, 790-8577, Japan

SOURCE: Heterocycles (2006), 67(1), 255-267

CODEN: HTCYAM; ISSN: 0385-5414

PUBLISHER: Japan Institute of Heterocyclic Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 144:323611

AB Zinc benzoporphyrins fused with one acenaphthylene or fluoranthene, (3) and (4) resp., were prepared by the condensation of a bicyclo[2.2.2]octadiene (BCOD)-fused tripyrrane with appropriate pyrrole dialdehydes and the subsequent retro Diels-Alder reaction. The absorptions of these new porphyrins were very intense at both Soret and Q bands, which might be useful as organic dyes for solar cells.

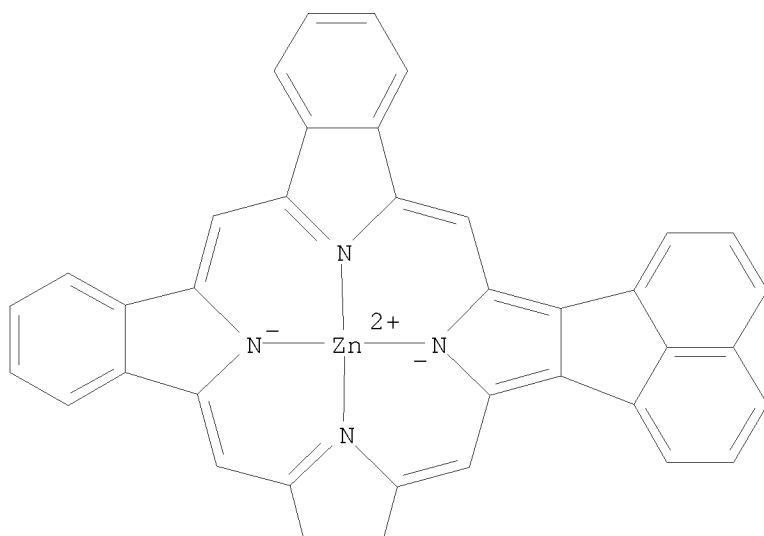
IT 879896-29-4P 880171-42-6P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (new preparation of zinc complexes of benzoporphyrins fused with acenaphthylene or fluoranthene, and absorption spectra as potential dyes for solar cells)

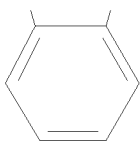
RN 879896-29-4 CAPLUS

CN Zinc, [31H,33H-acenaphtho[1,2-b]tribenzo[g,l,q]porphinato(2-)-κN31,κN32,κN33,κN34]-, (SP-4-1)- (9CI) (CA INDEX NAME)

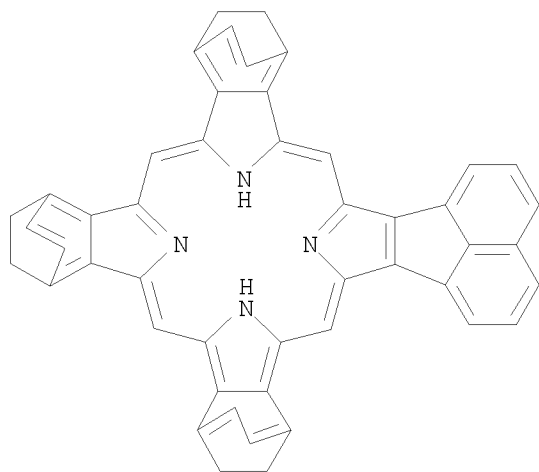
PAGE 1-A



PAGE 2-A



RN 880171-42-6 CAPLUS  
 CN 1,4:8,11:15,18-Triethano-31H,33H-acenaphtho[1,2-b]tribenzo[g,l,q]porphine  
 (9CI) (CA INDEX NAME)



REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 13 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2006:91919 CAPLUS

DOCUMENT NUMBER: 145:387119

TITLE: High performance porphyrin semiconductor for transistor applications

AUTHOR(S): Aramaki, Shinji; Yoshiyama, Ruichi; Sakai, Masayoshi; Ono, Noboru

CORPORATE SOURCE: Mitsubishi Chemical Group Science & Technology Research Center, Inc., 1000 Kamoshida-cho, Aoba-ku, Yokohama, 227-8502, Japan

SOURCE: Digest of Technical Papers - Society for Information Display International Symposium (2005), 36(Bk. 1), 296-299

CODEN: DTPSDS

PUBLISHER: Society for Information Display

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Various porphyrin compds. were investigated for solution-processible semiconductors for transistor applications. Some show excellent semiconductor properties. Their films can be formed by solution-process, i.e., by thermal conversion of their precursor film coated from their solution. Some porphyrin compds. show good semiconductor performance in terms of mobility and long-term driving stability.

IT 910923-74-9

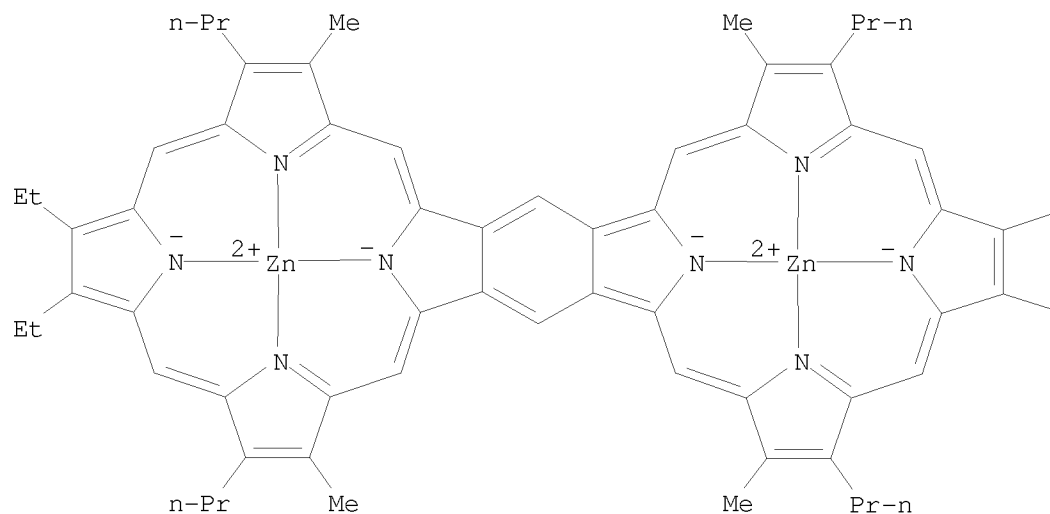
RL: DEV (Device component use); PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); PROC (Process); USES (Uses)

(high performance porphyrin semiconductor for transistor applications)

RN 910923-74-9 CAPLUS

CN Zinc, [ $\mu$ -[9,10,28,29-tetraethyl-4,15,23,34-tetramethyl-5,14,24,33-tetrapropyl-39H,41H,43H,45H-benzo[1,2-b:4,5-b']diporphinato(4-)- $\kappa$ N39, $\kappa$ N40, $\kappa$ N41, $\kappa$ N42: $\kappa$ N43, $\kappa$ N44, $\kappa$ N45, $\kappa$ N46]]di- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B

Et

Et

REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 14 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2005:1198904 CAPLUS  
 DOCUMENT NUMBER: 144:88067  
 TITLE: Porphyrins with exocyclic rings. Part 19: Efficient syntheses of phenanthrolineporphyrins  
 AUTHOR(S): Lash, Timothy D.; Lin, Yanning; Novak, Bennett H.; Parikh, Mihir D.  
 CORPORATE SOURCE: Department of Chemistry, Illinois State University, Normal, IL, 61790-4160, USA  
 SOURCE: Tetrahedron (2005), 61(49), 11601-11614  
 CODEN: TETRAB; ISSN: 0040-4020  
 PUBLISHER: Elsevier B.V.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

OTHER SOURCE(S): CASREACT 144:88067  
GI

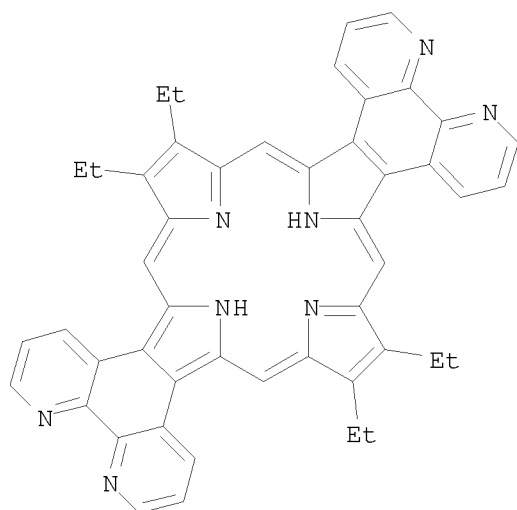
\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB 5-Nitro-1,10-phenanthrolines react with isocyanoacetate esters in the presence of DBU in THF to give excellent yields of the corresponding phenanthrolinopyrroles, e. g. I. These were condensed with acetoxymethylpyrroles using catalytic quantities of p-toluenesulfonic acid in acetic acid to give dipyrromethanes, e.g. II, but these structures proved to be poorly suited for porphyrin synthesis due to the electron-withdrawing nature of the fused phenanthroline unit. However, phenanthrolinopyrrole Et esters could be converted to the corresponding  $\alpha$ -unsubstituted pyrroles with KOH in ethylene glycol at 180-190 °C, and these condensed with 2 equiv of acetoxymethylpyrroles in refluxing acetic acid-iso-Pr alc. to give tripyrranes, e.g. III. In a one pot procedure, tripyrrane di-tert-Bu esters were treated with TFA at room temperature to cleave the protective groups, diluted with dichloromethane, reacted with pyrrole dialdehydes and oxidized to afford phenanthrolinoporphyrins, e.g. IV, in 52-83% yield. These conditions also allow the synthesis of porphyrins with addnl. fused acenaphthylene or phenanthrene rings. Although the UV-vis spectra for these porphyrins are unexceptional, the presence of an external coordination site allows many potential applications to be considered. Porphyrins with two phenanthroline units could not be prepared by the '3+1' strategy. Instead,  $\alpha$ -unsubstituted phenanthrolinopyrroles were reacted with a bis(dimethylaminomethyl)pyrrole in refluxing acetic acid to give moderate yields of the corresponding opp-diphenanthrolinoporphyrins. In one case, a triphenanthrolinoporphyrin and trace amts. of an adj-diphenanthrolinoporphyrin were formed as byproducts.

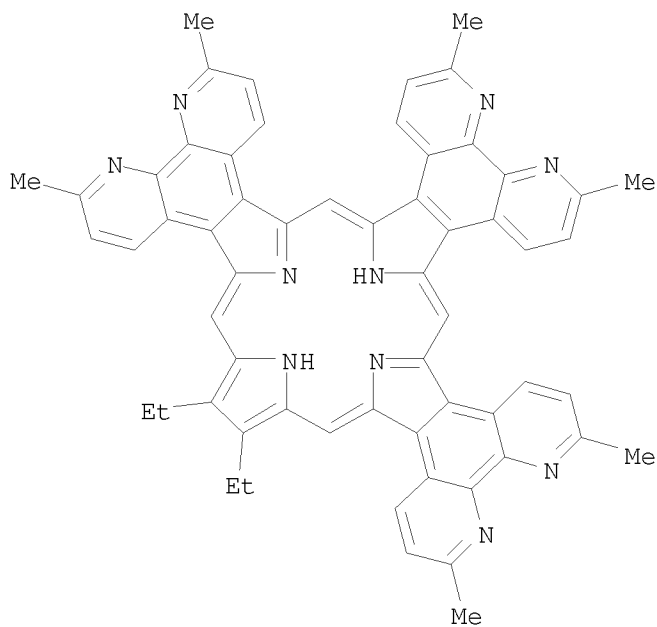
IT 872452-65-8P 872452-66-9P 872452-75-0P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(efficient syntheses of phenanthrolinoporphyrins)

RN 872452-65-8 CAPLUS

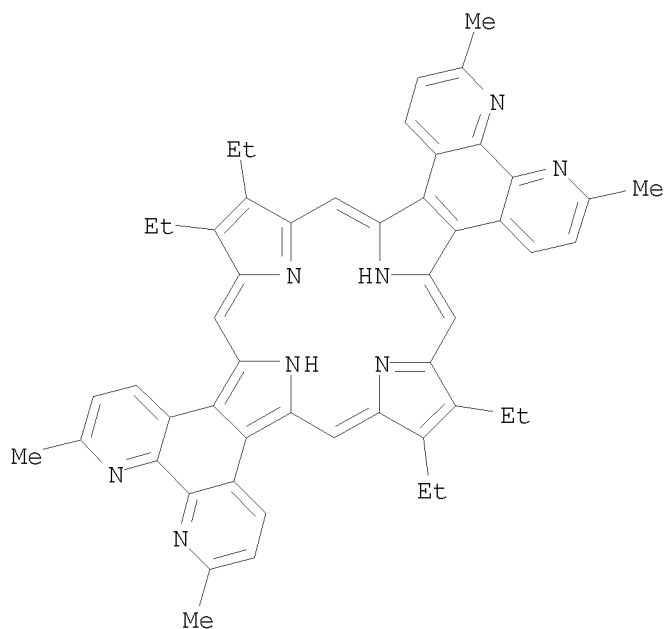
CN 33H,35H-Di[1,10]phenanthrolino[5,6-b:5',6'-1]porphine,  
12,13,28,29-tetraethyl- (9CI) (CA INDEX NAME)



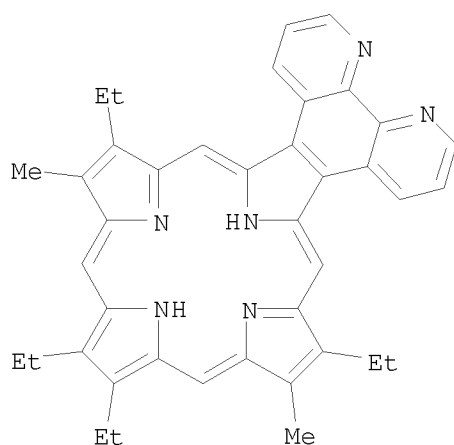
RN 872452-66-9 CAPLUS  
 CN 39H,41H-Tri[1,10]phenanthrolino[5,6-b:5',6''-g:5''',6'''-l]porphine,  
 19,20-diethyl-2,10,13,26,29,37-hexamethyl- (9CI) (CA INDEX NAME)



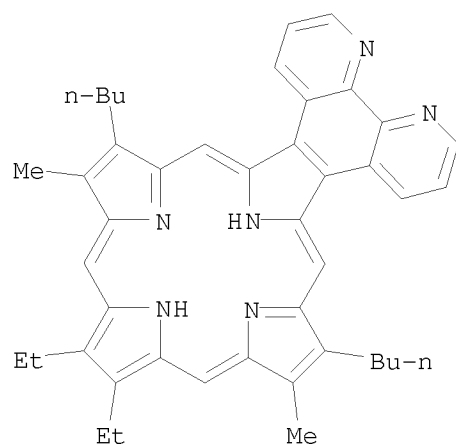
RN 872452-75-0 CAPLUS  
 CN 33H,35H-Di[1,10]phenanthrolino[5,6-b:5',6''-l]porphine,  
 12,13,28,29-tetraethyl-3,6,19,22-tetramethyl- (9CI) (CA INDEX NAME)



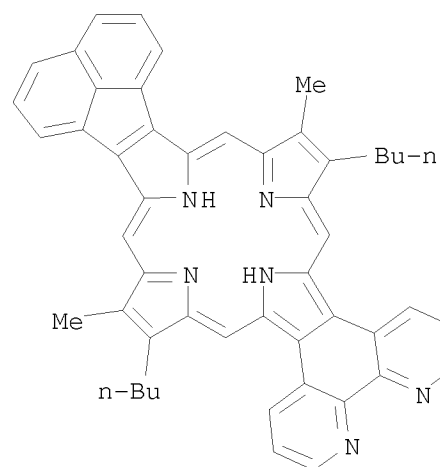
IT 172806-00-7P 172806-03-0P 872452-63-6P  
 872452-64-7P 872452-74-9P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (efficient syntheses of phenanthrolineporphyrins)  
 RN 172806-00-7 CAPLUS  
 CN 27H,29H-[1,10]Phenanthroline[5,6-b]porphine,  
 12,17,18,23-tetraethyl-13,22-dimethyl- (9CI) (CA INDEX NAME)



RN 172806-03-0 CAPLUS  
 CN 27H,29H-[1,10]Phenanthroline[5,6-b]porphine,  
 12,23-dibutyl-17,18-diethyl-13,22-dimethyl- (9CI) (CA INDEX NAME)

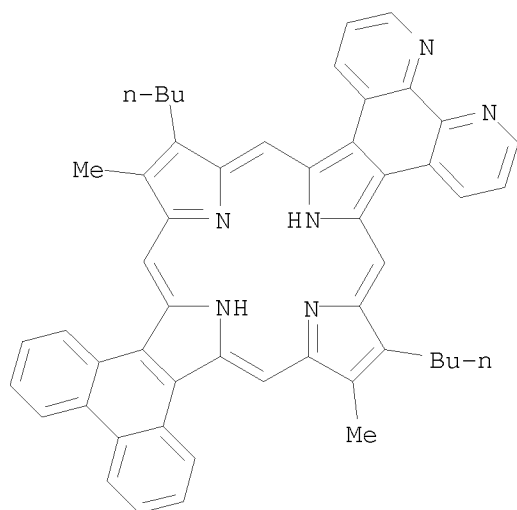


RN 872452-63-6 CAPLUS  
 CN 31H,33H-Acenaphtho[1,2-b][1,10]phenanthrolino[5,6-l]porphine,  
 12,27-dibutyl-13,26-dimethyl- (9CI) (CA INDEX NAME)

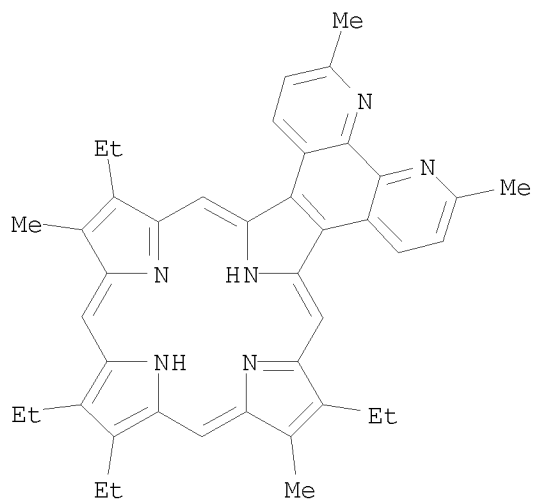


RN 872452-64-7 CAPLUS  
 CN 33H,35H-Phenanthro[9,10-b][1,10]phenanthrolino[5,6-l]porphine,  
 12,29-dibutyl-13,28-dimethyl- (9CI) (CA INDEX NAME)





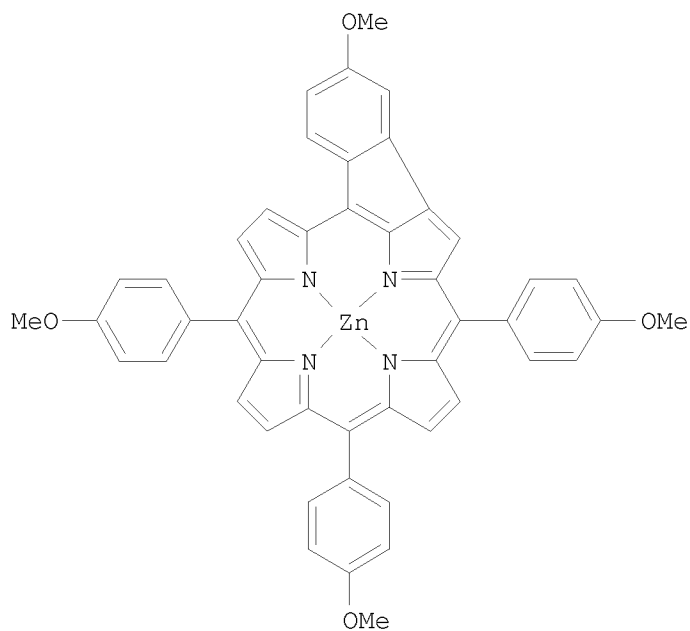
RN 872452-74-9 CAPLUS  
 CN 27H,29H-[1,10]Phenanthroline[5,6-b]porphine,  
 12,17,18,23-tetraethyl-3,6,13,22-tetramethyl- (9CI) (CA INDEX NAME)



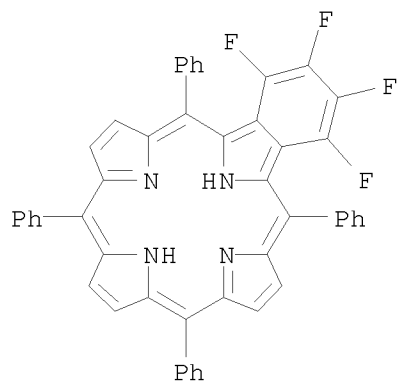
REFERENCE COUNT: 108 THERE ARE 108 CITED REFERENCES AVAILABLE FOR  
 THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE  
 FORMAT

L9 ANSWER 15 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2005:1060945 CAPLUS  
 DOCUMENT NUMBER: 144:31616  
 TITLE: A novel and facile Zn-mediated intramolecular  
 five-membered cyclization of  $\beta$ -tetraarylporphyrin  
 radicals from  $\beta$ -bromotetraarylporphyrins  
 AUTHOR(S): Shen, Dong-Mei; Liu, Chao; Chen, Qing-Yun  
 CORPORATE SOURCE: Key Laboratory of Organofluorine Chemistry, Shanghai

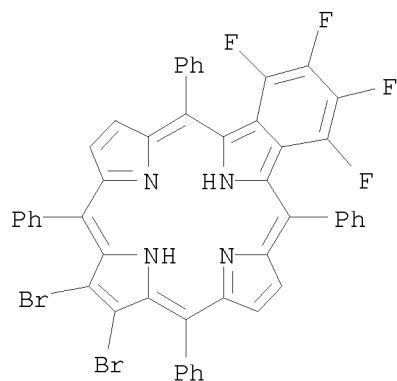
SOURCE: Institute of Organic Chemistry, Chinese Academy of Sciences, 354 Fenglin Road, 200032, Peop. Rep. China  
 Chemical Communications (Cambridge, United Kingdom) (2005), (39), 4982-4984  
 CODEN: CHCOFS; ISSN: 1359-7345  
 PUBLISHER: Royal Society of Chemistry  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 144:31616  
 GI



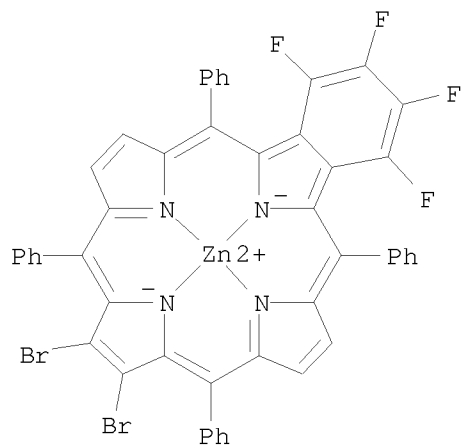
AB A novel and facile method for the Zn-mediated intramol. cyclization of  $\beta$ -porphyrin radicals has been developed for the convenient and effective construction of newly fused five-membered porphyrin systems from readily available  $\beta$ -bromotetraarylporphyrins. Reacting the Zn-coordinated porphyrins with Zn/DMSO gave the cyclized product, e.g. I.  
 IT 848394-52-5  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (Zn-mediated intramol. cyclization of  $\beta$ -bromotetraarylporphyrins)  
 RN 848394-52-5 CAPLUS  
 CN 23H,25H-Benzo[b]porphine, 1,2,3,4-tetrafluoro-6,11,16,21-tetraphenyl- (CA INDEX NAME)



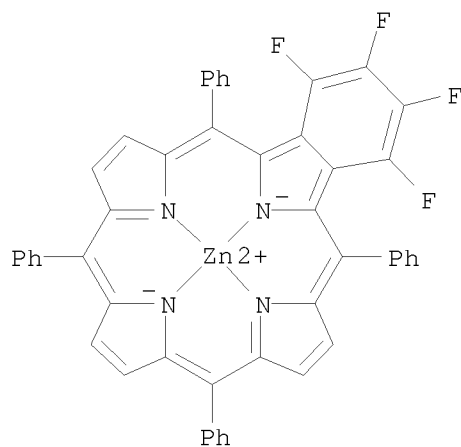
IT 870251-21-1P 870251-39-1P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (Zn-mediated intramol. cyclization of  $\beta$ -bromotetraarylporphyrins)  
 RN 870251-21-1 CAPLUS  
 CN 23H,25H-Benzo[b]porphine, 13,14-dibromo-1,2,3,4-tetrafluoro-6,11,16,21-tetraphenyl- (9CI) (CA INDEX NAME)



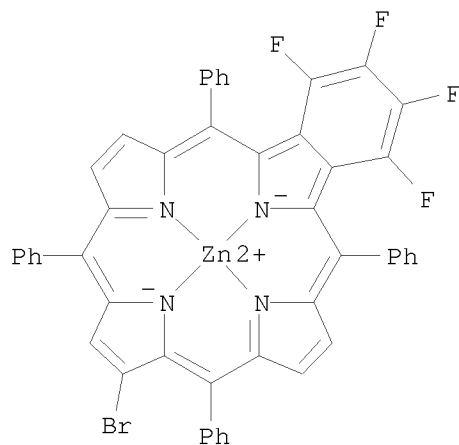
RN 870251-39-1 CAPLUS  
 CN Zinc, [13,14-dibromo-1,2,3,4-tetrafluoro-6,11,16,21-tetraphenyl-23H,25H-benzo[b]porphinato(2-)- $\kappa$ N23, $\kappa$ N24, $\kappa$ N25, $\kappa$ N26]-, (SP-4-1)- (9CI) (CA INDEX NAME)



IT 848394-49-0P 870251-23-3P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (Zn-mediated intramol. cyclization of  $\beta$ -bromotetraarylporphyrins)  
 RN 848394-49-0 CAPLUS  
 CN Zinc, [1,2,3,4-tetrafluoro-6,11,16,21-tetraphenyl-23H,25H-benzo[b]porphinato(2-)- $\kappa$ N23, $\kappa$ N24, $\kappa$ N25, $\kappa$ N26]-, (SP-4-1)- (CA INDEX NAME)



RN 870251-23-3 CAPLUS  
 CN Zinc, [13-bromo-1,2,3,4-tetrafluoro-6,11,16,21-tetraphenyl-23H,25H-benzo[b]porphinato(2-)- $\kappa$ N23, $\kappa$ N24, $\kappa$ N25, $\kappa$ N26]-, (SP-4-2)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 16 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2005:1024795 CAPLUS  
 DOCUMENT NUMBER: 143:487781  
 TITLE: Diels-Alder reactions of pyrrolo[3,4-b]porphyrins  
 AUTHOR(S): Liu, Wei; Fronczek, Frank R.; Vicente, M. Graca H.;  
 Smith, Kevin M.  
 CORPORATE SOURCE: Department of Chemistry, Louisiana State University,  
 Baton Rouge, LA, 70803, USA  
 SOURCE: Tetrahedron Letters (2005), 46(43), 7321-7324  
 CODEN: TELEAY; ISSN: 0040-4039  
 PUBLISHER: Elsevier B.V.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 143:487781  
 GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

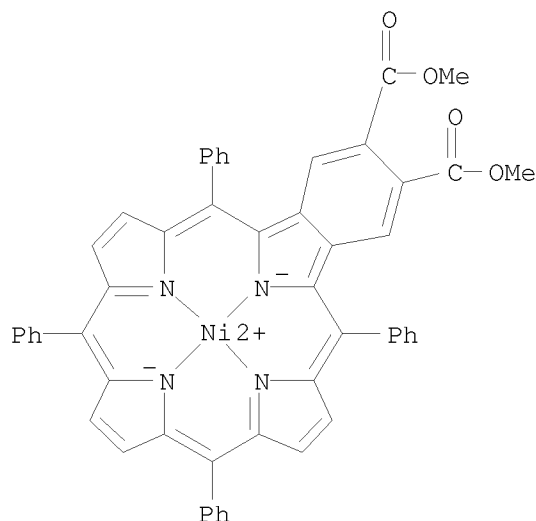
AB In the presence of excess dimethylacetylene dicarboxylate (DMAD), Ni(II) pyrrolo[3,4-b]porphyrins undergo both Diels-Alder cycloaddn. and Michael addition in toluene to give two bis-adducts, identified as compds. I and II; the reaction can be accelerated by the addition of Lewis or Bronsted-Lowry acids. Refluxing the reaction mixture in 1,2,4-trichlorobenzene (220°) leads to a Ni(II) monobenzoporphyrin as the main product. The structure of compound I was confirmed by x-ray crystallog.

IT 255366-66-6P  
 RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); SPN (Synthetic preparation); PREP (Preparation); PROC (Process) (preparation from Diels-Alder cycloaddn. and Michael addition of nickel pyrroloporphyrin with dimethylacetylene dicarboxylate)

RN 255366-66-6 CAPLUS

CN Nickel, [dimethyl 6,11,16,21-tetraphenyl-23H,25H-benzo[b]porphine-2,3-

dicarboxylato(2-)-κN23, κN24, κN25, κN26]-, (SP-4-1)-  
(9CI) (CA INDEX NAME)



REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 17 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2005:645336 CAPLUS  
 DOCUMENT NUMBER: 143:317778  
 TITLE: Enlarged  $\pi$ -electronic network of a meso-meso,  $\beta$ - $\beta$ ,  $\beta$ - $\beta$  triply linked dibenzoporphyrin dimer that exhibits a large two-photon absorption cross section  
 AUTHOR(S): Inokuma, Yasuhide; Ono, Noboru; Uno, Hidemitsu; Kim, Deok Yun; Noh, Soo Bum; Kim, Dongho; Osuka, Atsuhiko  
 CORPORATE SOURCE: Department of Chemistry, Graduate School of Science, Kyoto University, Sakyo-ku, Kyoto, 606-8502, Japan  
 SOURCE: Chemical Communications (Cambridge, United Kingdom) (2005), (30), 3782-3784  
 CODEN: CHCOFS; ISSN: 1359-7345  
 PUBLISHER: Royal Society of Chemistry  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 143:317778  
 GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB Enlargement of the  $\pi$ -electronic network of meso-meso,  $\beta$ - $\beta$ ,  $\beta$ - $\beta$  triply linked diporphyrin was exploited by preparing a corresponding dibenzo-fused porphyrin dimer that exhibits a perturbed absorption spectrum and a large two-photon absorption cross section. The dibenzo-fused porphyrin dimer (I; Ar = 4-tert-butylphenyl) was prepared from

the monomeric zinc porphyrin derivative (II) via coupling and retro Diels-Alder reactions. The crystal structure of the meso-meso singly linked dimeric zinc dibenzoporphyrin precursor of complex I was determined. The electrochem. properties of these complexes were also examined.

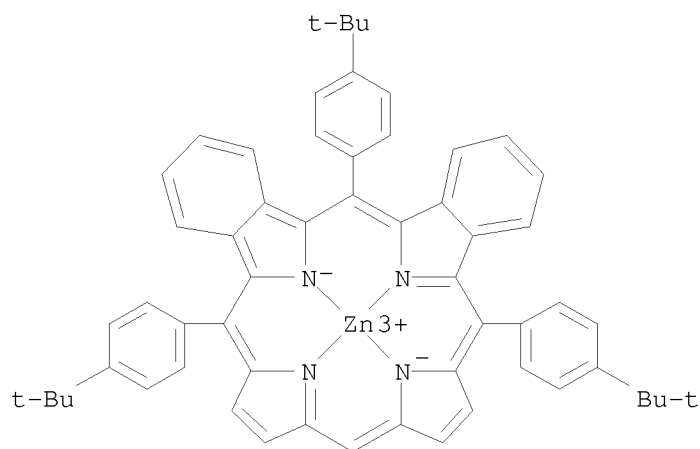
IT 864919-90-4 864919-91-5 864919-96-0  
864919-97-1 864919-98-2 864919-99-3  
864920-00-3 864920-01-4 864920-02-5  
864920-03-6

RL: CPS (Chemical process); FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); FORM (Formation, nonpreparative); PROC (Process)

(elec. potential of couple containing)

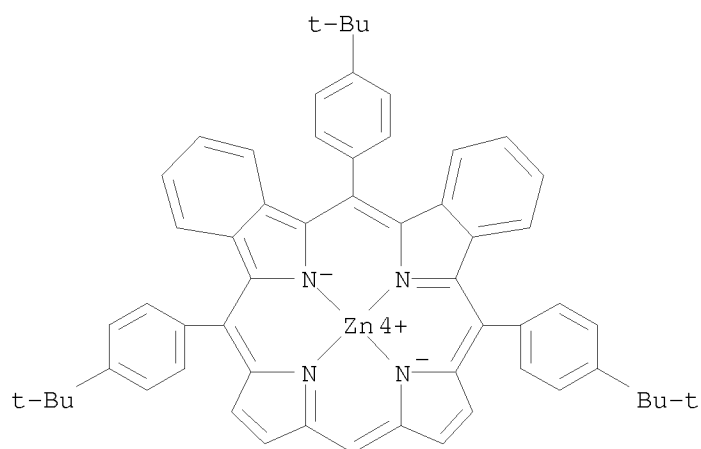
RN 864919-90-4 CAPLUS

CN Zinc(1+), [5,10,15-tris[4-(1,1-dimethylethyl)phenyl]-21H,23H-porphinato(2-)-κN21,κN22,κN23,κN24]-, (SP-4-2)- (9CI) (CA INDEX NAME)



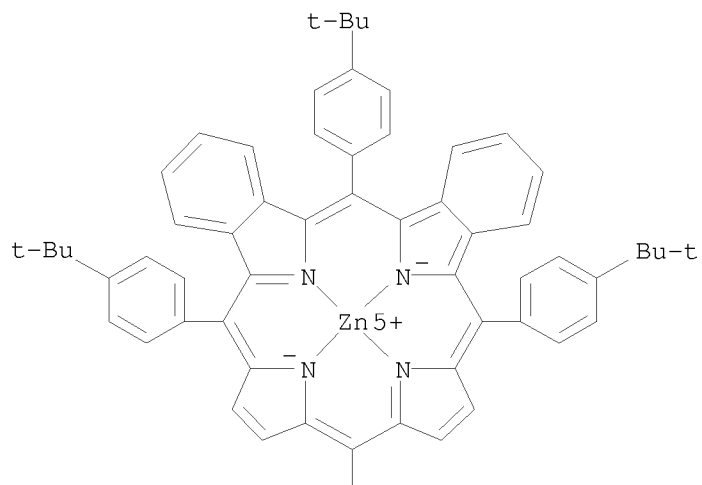
RN 864919-91-5 CAPLUS

CN Zinc(2+), [5,10,15-tris[4-(1,1-dimethylethyl)phenyl]-21H,23H-porphinato(2-)-κN21,κN22,κN23,κN24]-, (SP-4-2)- (9CI) (CA INDEX NAME)



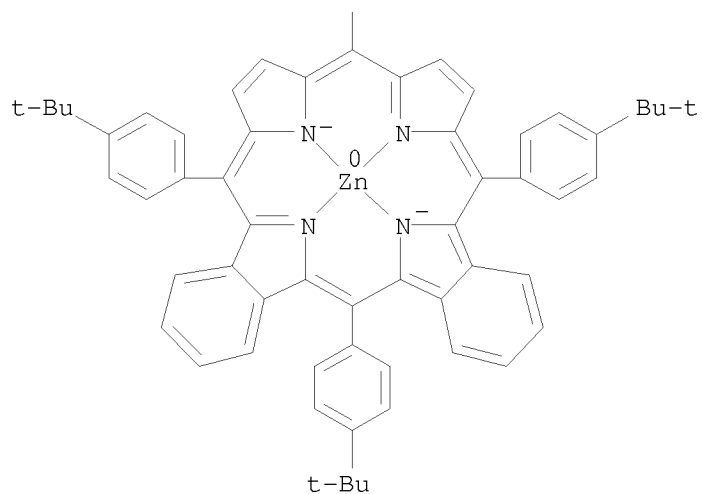
RN 864919-96-0 CAPLUS  
 CN Zinc(1+), [ $\mu$ -[6,6',16,16',23,23'-hexakis[4-(1,1-dimethylethyl)phenyl]-11,11'-bi-25H,27H-dibenzo[b,g]porphinato(4-)- $\kappa\text{N}25,\kappa\text{N}26,\kappa\text{N}27,\kappa\text{N}28:\kappa\text{N}25',\kappa\text{N}26',\kappa\text{N}27',\kappa\text{N}28']$ di- (9CI) (CA INDEX NAME)

PAGE 1-A



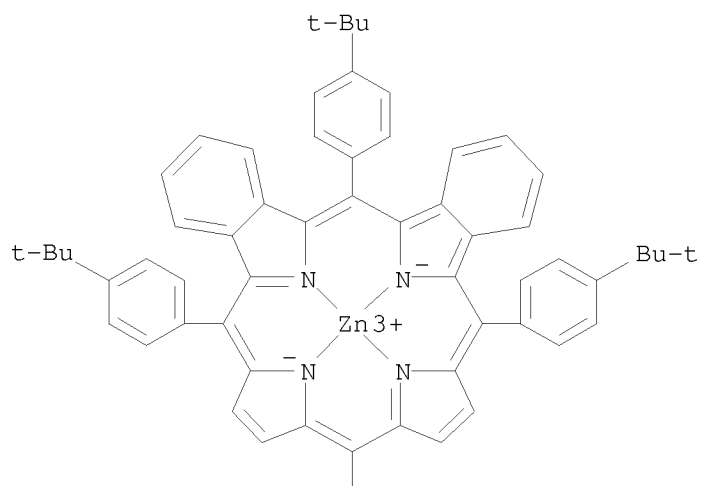


PAGE 2-A

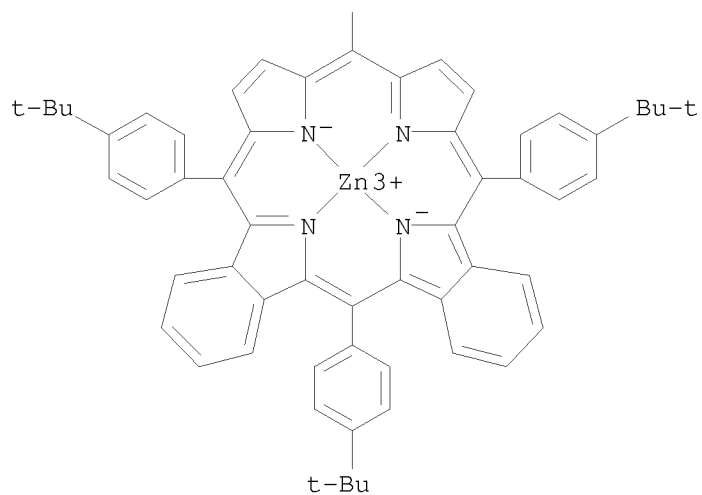


RN 864919-97-1 CAPLUS  
 CN Zinc(2+), [ $\mu$ -[6,6',16,16',23,23'-hexakis[4-(1,1-dimethylethyl)phenyl]-11,11'-bi-25H,27H-dibenzo[b,g]porphinato(4-)- $\kappa$ N25, $\kappa$ N26, $\kappa$ N27, $\kappa$ N28: $\kappa$ N25', $\kappa$ N26', $\kappa$ N27', $\kappa$ N28']]di- (9CI) (CA INDEX NAME)

PAGE 1-A

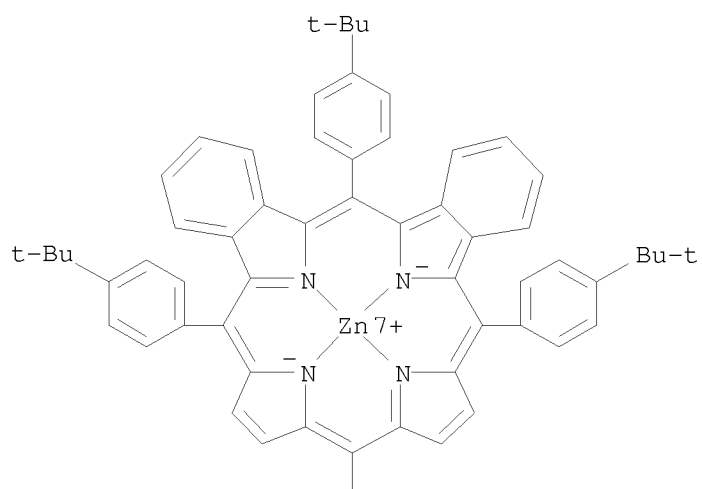


PAGE 2-A

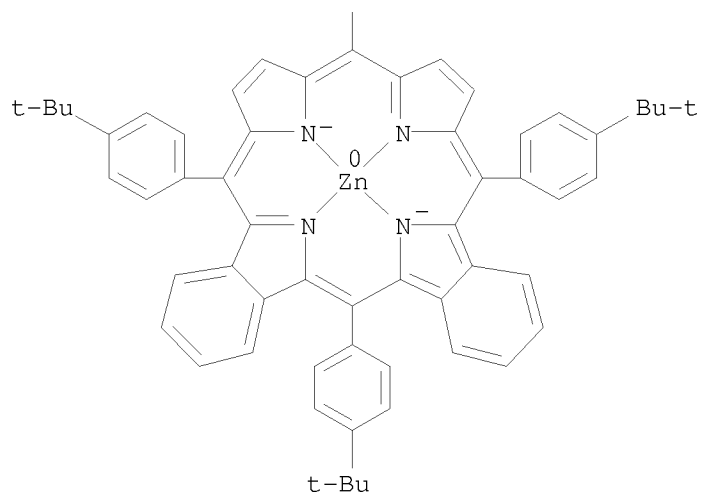


RN 864919-98-2 CAPLUS  
 CN Zinc(3+), [ $\mu$ -[6,6',16,16',23,23'-hexakis[4-(1,1-dimethylethyl)phenyl]-11,11'-bi-25H,27H-dibenzo[b,g]porphinato(4-)- $\kappa$ N25, $\kappa$ N26, $\kappa$ N27, $\kappa$ N28: $\kappa$ N25', $\kappa$ N26', $\kappa$ N27', $\kappa$ N28']]di- (9CI) (CA INDEX NAME)

PAGE 1-A

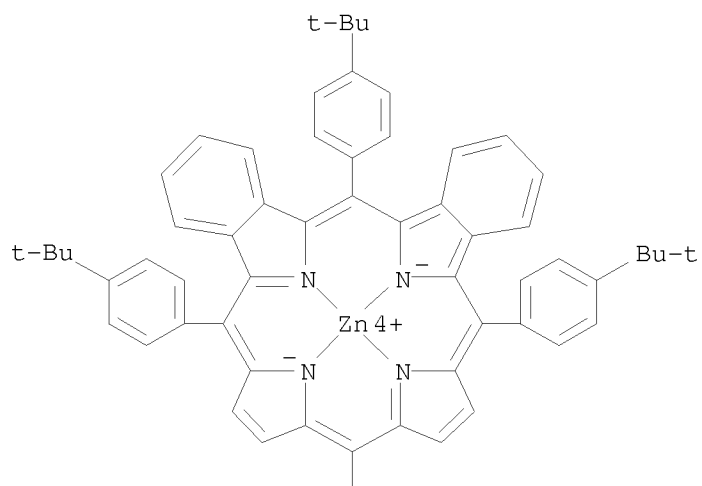


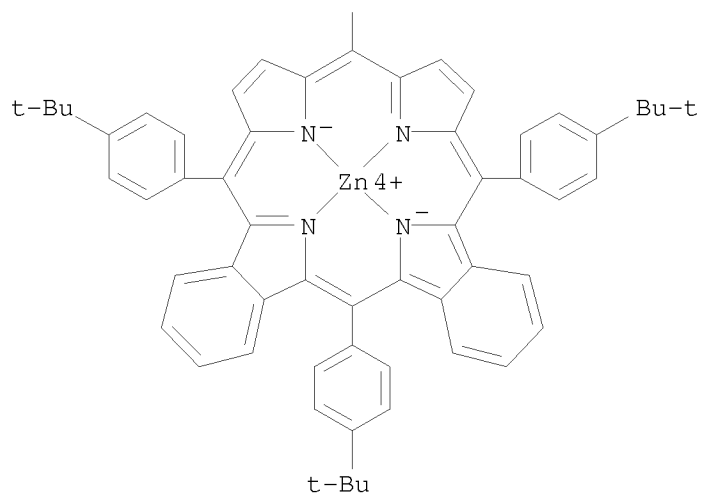
PAGE 2-A



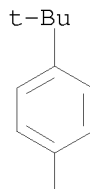
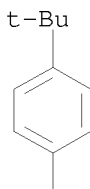
RN 864919-99-3 CAPLUS  
 CN Zinc(4+), [ $\mu$ -[6,6',16,16',23,23'-hexakis[4-(1,1-dimethylethyl)phenyl]-11,11'-bi-25H,27H-dibenzo[b,g]porphinato(4-)- $\kappa$ N25, $\kappa$ N26, $\kappa$ N27, $\kappa$ N28: $\kappa$ N25', $\kappa$ N26', $\kappa$ N27', $\kappa$ N28']] $\mu$ -di- (9CI) (CA INDEX NAME)

PAGE 1-A





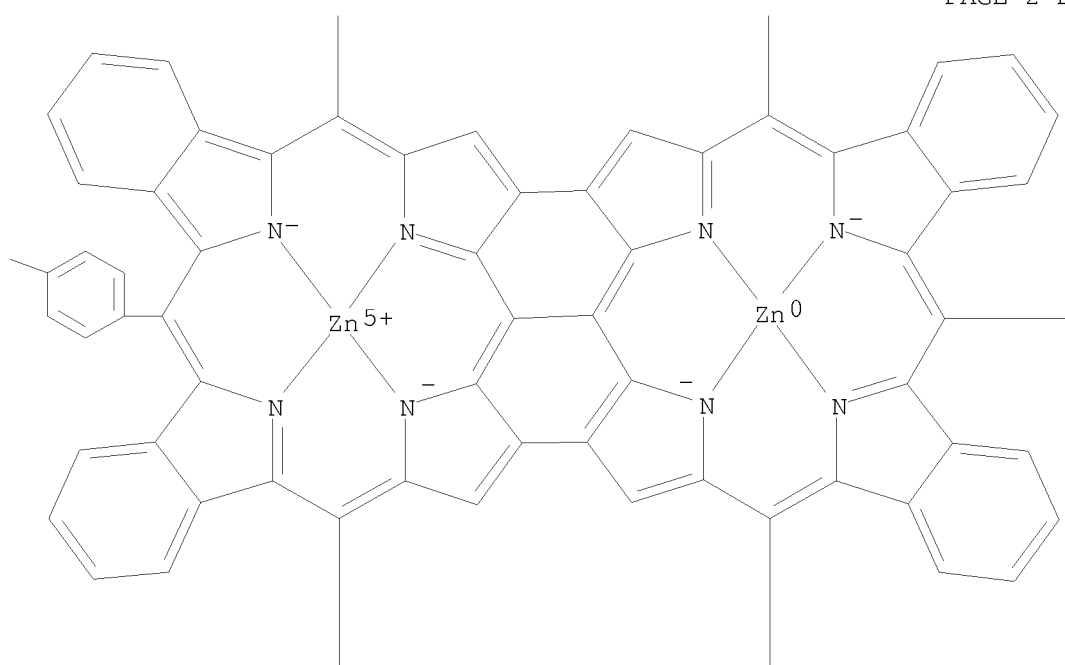
RN 864920-00-3 CAPLUS  
 CN Zinc(1+), [ $\mu$ -[6,6',16,16',23,23'-hexakis[4-(1,1-dimethylethyl)phenyl]-9,9':11,11':13,13'-bis(25H,27H-dibenzo[b,g]porphinato)(4-)- $\kappa$ N25, $\kappa$ N26, $\kappa$ N27, $\kappa$ N28: $\kappa$ N25', $\kappa$ N26', $\kappa$ N27', $\kappa$ N28']]di- (9CI) (CA INDEX NAME)



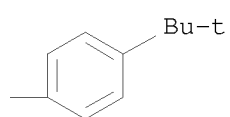
PAGE 2-A

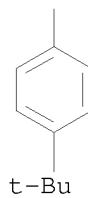
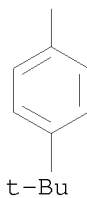
t-Bu

PAGE 2-B



PAGE 2-C

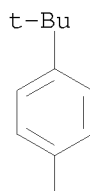
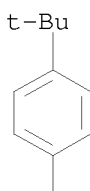




PAGE 3-B

RN 864920-01-4 CAPLUS  
 CN Zinc(2+), [ $\mu$ -[6,6',16,16',23,23'-hexakis[4-(1,1-dimethylethyl)phenyl]-9,9':11,11':13,13'-bis(25H,27H-dibenzo[b,g]porphinato)(4-)- $\kappa$ N25, $\kappa$ N26, $\kappa$ N27, $\kappa$ N28: $\kappa$ N25', $\kappa$ N26',.kappa.N27', $\kappa$ N28']]]di- (9CI) (CA INDEX NAME)

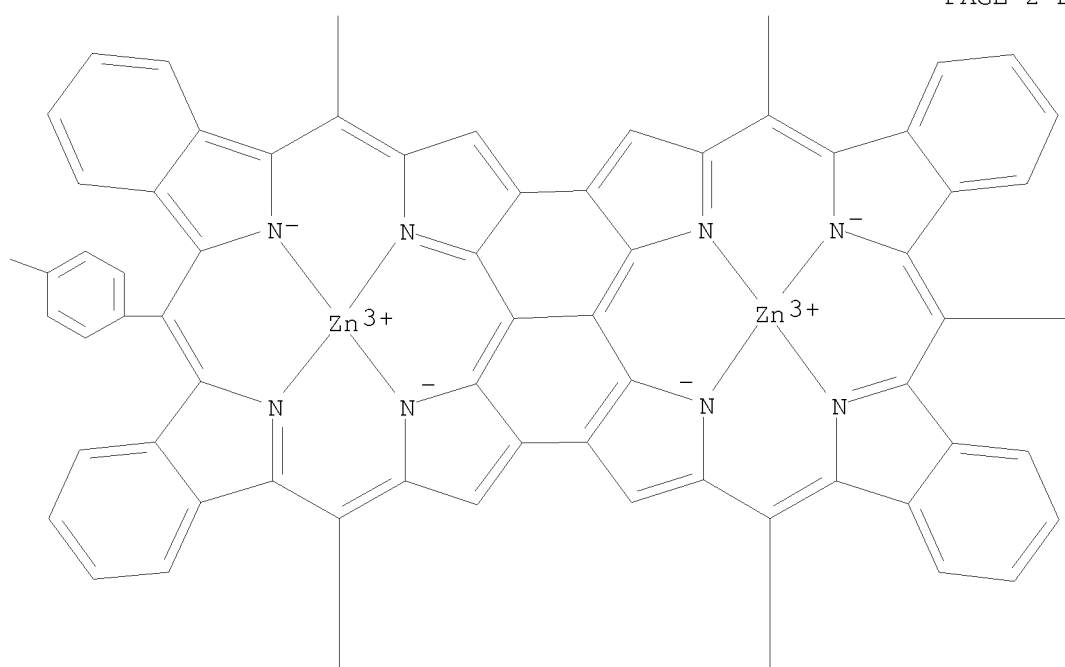
PAGE 1-B



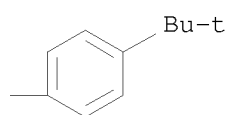
PAGE 2-A

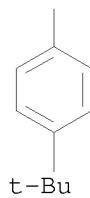
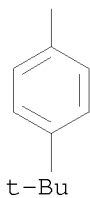
t-Bu

PAGE 2-B



PAGE 2-C

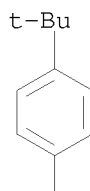
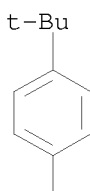




PAGE 3-B

RN 864920-02-5 CAPLUS  
 CN Zinc(3+), [ $\mu$ -[6,6',16,16',23,23'-hexakis[4-(1,1-dimethylethyl)phenyl]-9,9':11,11':13,13'-bis(25H,27H-dibenzo[b,g]porphinato)(4-)- $\kappa$ N25, $\kappa$ N26, $\kappa$ N27, $\kappa$ N28: $\kappa$ N25', $\kappa$ N26',.kappa.N27', $\kappa$ N28']]]di- (9CI) (CA INDEX NAME)

PAGE 1-B

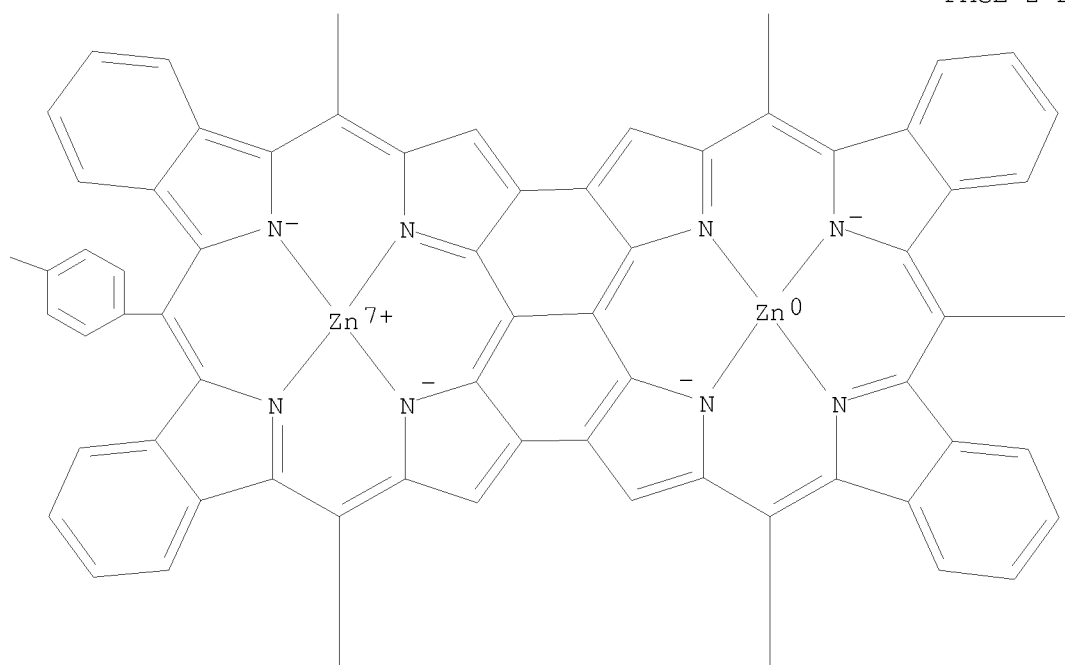




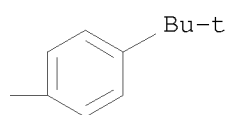
PAGE 2-A

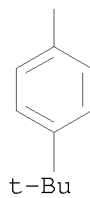
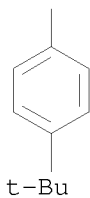
t-Bu

PAGE 2-B



PAGE 2-C

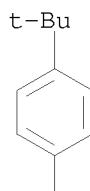
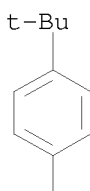




PAGE 3-B

RN 864920-03-6 CAPLUS  
 CN Zinc(4+), [ $\mu$ -[6,6',16,16',23,23'-hexakis[4-(1,1-dimethylethyl)phenyl]-  
 9,9':11,11':13,13'-bis(25H,27H-dibenzo[b,g]porphinato)(4-)-  
 $\kappa$ N25, $\kappa$ N26, $\kappa$ N27, $\kappa$ N28: $\kappa$ N25', $\kappa$ N26',.kappa  
 .N27', $\kappa$ N28']]di- (9CI) (CA INDEX NAME)

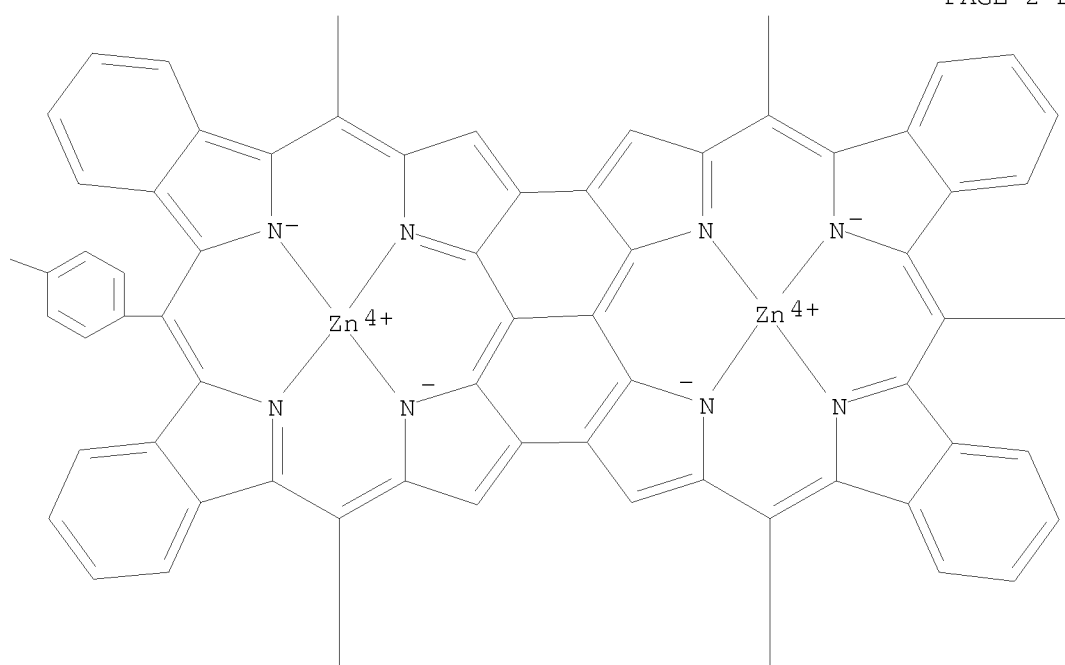
PAGE 1-B



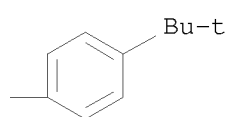
PAGE 2-A

t-Bu

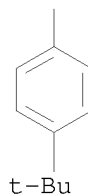
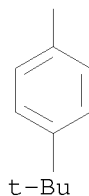
PAGE 2-B



PAGE 2-C

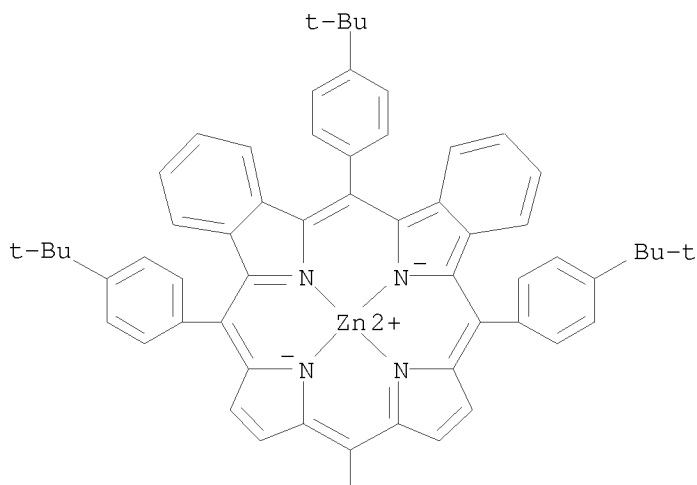


PAGE 3-B

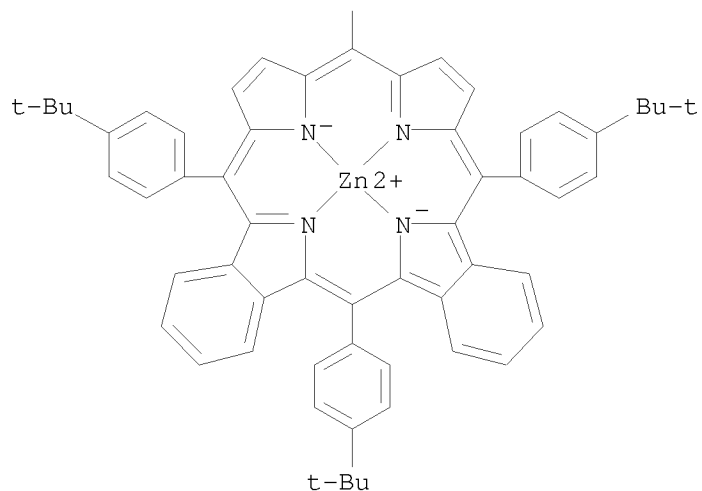


IT 864919-87-9P  
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
 (preparation and crystal structure of meso-meso singly linked zinc  
 dibenzoporphyrin dimer)  
 RN 864919-87-9 CAPLUS  
 CN Zinc, [ $\mu$ -[6,6',16,16',23,23'-hexakis[4-(1,1-dimethylethyl)phenyl]-  
 11,11'-bi-25H,27H-dibenzo[b,g]porphinato(4-)-  
 $\kappa$ N25, $\kappa$ N26, $\kappa$ N27, $\kappa$ N28: $\kappa$ N25', $\kappa$ N26',.kappa  
 .N27', $\kappa$ N28']]di-, compd. with pyridine (1:2) (9CI) (CA INDEX NAME)  
 CM 1  
 CRN 864919-85-7  
 CMF C116 H102 N8 Zn2  
 CCI CCS

PAGE 1-A



PAGE 2-A



CM 2

CRN 110-86-1

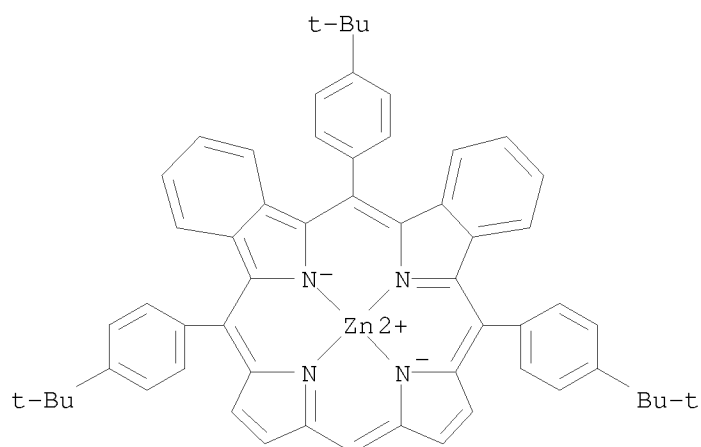
CMF C5 H5 N



IT 864919-82-4P  
 RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)  
 (preparation and electrochem. properties of monomeric zinc dibenzoporphyrin)

RN 864919-82-4 CAPLUS

CN Zinc, [5,10,15-tris[4-(1,1-dimethylethyl)phenyl]-21H,23H-porphinato(2-)- $\kappa$ N21, $\kappa$ N22, $\kappa$ N23, $\kappa$ N24]-, (SP-4-2)- (9CI) (CA INDEX NAME)

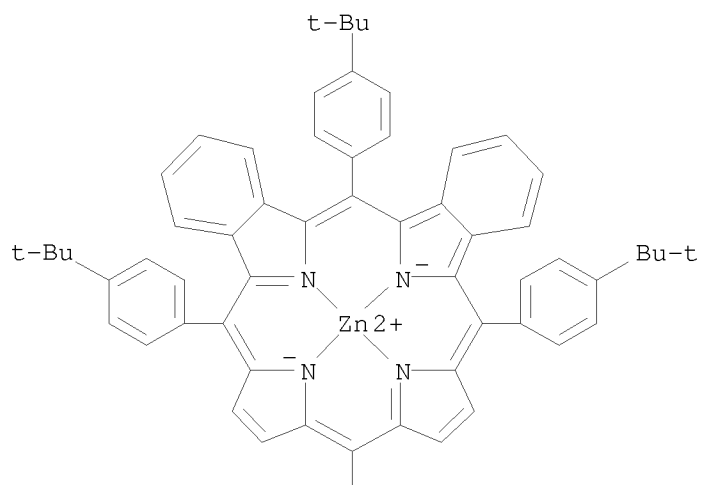


```

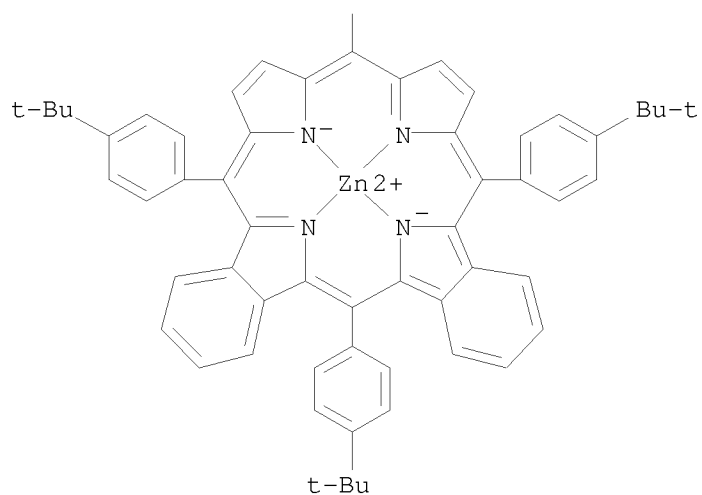
IT      864919-85-7P
      RL: CPS (Chemical process); PEP (Physical, engineering or chemical
      process); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation);
      PREP (Preparation); PROC (Process); RACT (Reactant or reagent)
      (preparation, electrochem. properties and coupling reaction for preparation
of
      zinc dibenzoporphyrin triply linked dimer)
RN      864919-85-7  CAPLUS
CN      Zinc,  [ $\mu$ -[6,6',16,16',23,23'-hexakis[4-(1,1-dimethylethyl)phenyl]-
      11,11'-bi-25H,27H-dibenzo[b,g]porphinato(4-)-
       $\kappa$ N25, $\kappa$ N26, $\kappa$ N27, $\kappa$ N28; $\kappa$ N25', $\kappa$ N26',.kappa
      .N27', $\kappa$ N28']di- (9CI)  (CA INDEX NAME)

```

PAGE 1-A



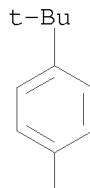
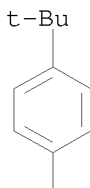
PAGE 2-A



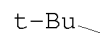
IT 864919-86-8P  
 RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)  
 (preparation, electrochem. properties and two-photon absorption spectrum of zinc dibenzoporphyrin triply linked dimer)  
 RN 864919-86-8 CAPLUS

CN Zinc, [ $\mu$ -[6,6',16,16',23,23'-hexakis[4-(1,1-dimethylethyl)phenyl]-9,9':11,11':13,13'-bis(25H,27H-dibenzo[b,g]porphinato) (4-)- $\kappa$ N25, $\kappa$ N26, $\kappa$ N27, $\kappa$ N28: $\kappa$ N25', $\kappa$ N26',.kappa.N27', $\kappa$ N28']]di- (9CI) (CA INDEX NAME)

PAGE 1-B

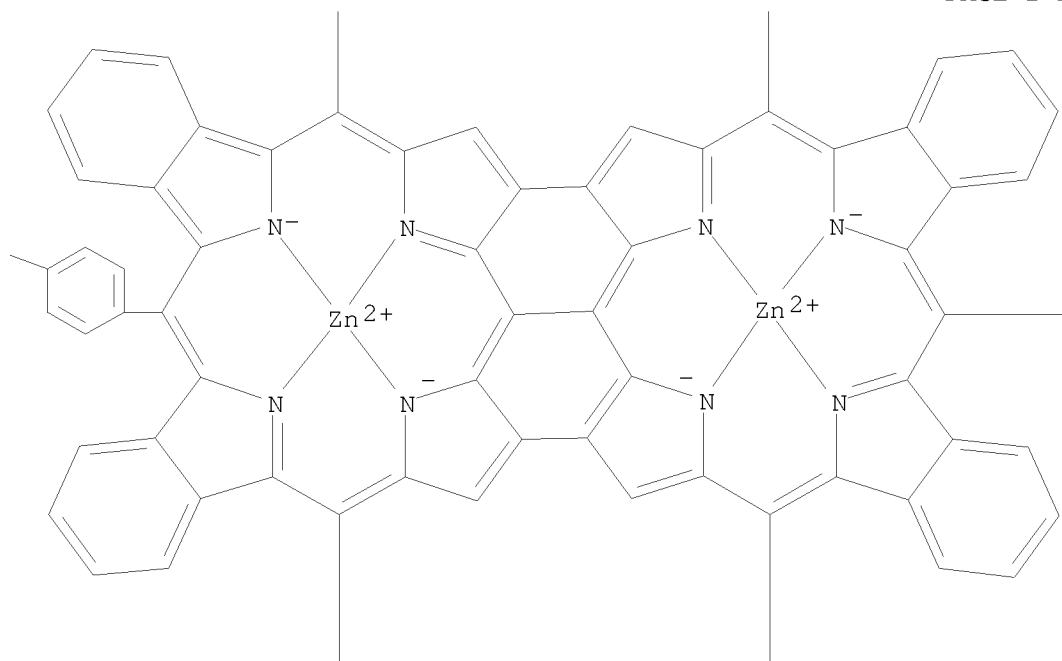


PAGE 2-A

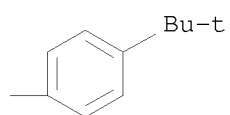




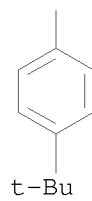
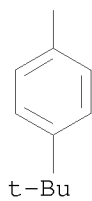
PAGE 2-B



PAGE 2-C



PAGE 3-B



REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS

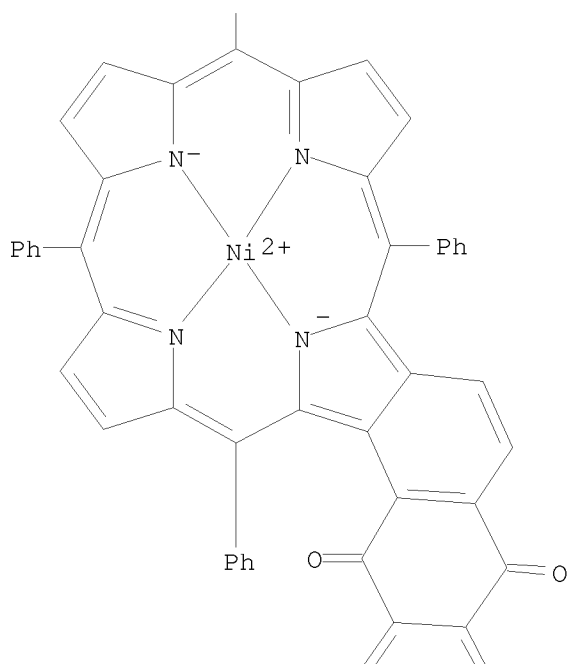
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 18 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2005:506595 CAPLUS  
 DOCUMENT NUMBER: 143:125238  
 TITLE: Diels-Alder reactions of  
 beta-vinyl-meso-tetraphenylporphyrin with quinones  
 AUTHOR(S): Faustino, Maria A. F.; Neves, Maria G. P. M. S.; Tome,  
 Augusto C.; Silva, Artur M. S.; Cavaleiro, Jose A. S.  
 CORPORATE SOURCE: Department of Chemistry, University of Aveiro, Aveiro,  
 3810-193, Port.  
 SOURCE: ARKIVOC (Gainesville, FL, United States) (2005), (9),  
 332-343  
 CODEN: AGFUAR  
 URL: [http://www.arkat-usa.org/ark/journal/2005/I09\\_Molina-Elguero/1324/ME-1324H.pdf](http://www.arkat-usa.org/ark/journal/2005/I09_Molina-Elguero/1324/ME-1324H.pdf)  
 PUBLISHER: Arkat USA Inc.  
 DOCUMENT TYPE: Journal; (online computer file)  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 143:125238  
 GI

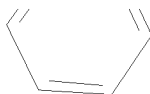
\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB Ni(II)-2-vinyl-5,10,15,20-tetraphenylporphyrin reacts with  
 1,4-naphthoquinone and 1,4-benzoquinone to afford mixts. of rigid  
 porphyrin-quinone derivs. (I-III and analogous benzoquinone derivs.,  
 resp.) with extended  $\pi$ -systems. The structures of these novel compds.  
 were deduced from detailed NMR expts.  
 IT 857254-04-7P 857254-05-8P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (preparation and demetalation of product of Diels-Alder reaction of  
 nickel(II) beta-vinyl-meso-tetraphenylporphyrin with naphthoquinone)  
 RN 857254-04-7 CAPLUS  
 CN Nickel, [2,7,12,17-tetraphenyl-27H,29H-anthra[1,2-b]porphine-21,26-  
 dionato(2-)- $\kappa$ N27, $\kappa$ N28, $\kappa$ N29, $\kappa$ N30]-, (SP-4-2)- (9CI)  
 (CA INDEX NAME)

Ph

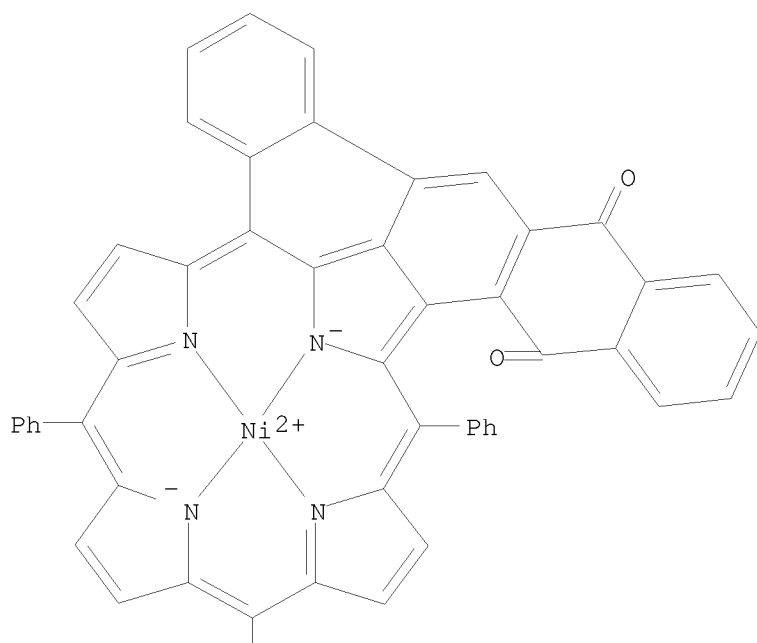


PAGE 3-A



RN 857254-05-8 CAPLUS  
 CN Nickel, [2,7,12-triphenyl-17,19[1',2']-benzeno-27H,29H-anthra[1,2-b]porphine-21,26-dionato(2-)-κN27,κN28,κN29,κN30]-, (SP-4-2)- (9CI) (CA INDEX NAME)

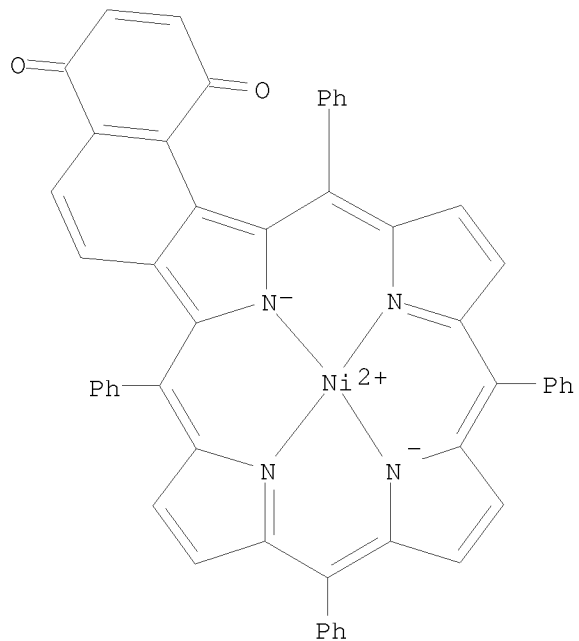
PAGE 1-A



PAGE 2-A

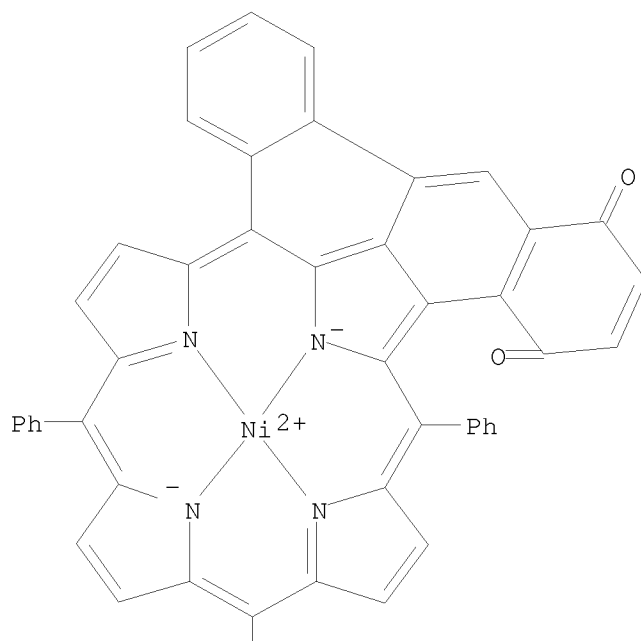


IT 857254-07-0P 857254-08-1P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation by Diels-Alder reaction of nickel(II)  
 beta-vinyl-meso-tetraphenylporphyrin with benzoquinone)  
 RN 857254-07-0 CAPLUS  
 CN Nickel, [8,13,18,23-tetraphenyl-25H,27H-naphtho[1,2-b]porphine-1,4-dionato(2-)-κN25,κN26,κN27,κN28]-, (SP-4-2)- (9CI)  
 (CA INDEX NAME)



RN 857254-08-1 CAPLUS  
 CN Nickel, [12,15,18-triphenyl-6,8[1',2']-benzeno-25H,27H-naphtho[1,2-b]porphine-1,4-dionato(2-)- $\kappa\text{N}25,\kappa\text{N}26,\kappa\text{N}27,\kappa\text{N}28$ ]-, (SP-4-2)- (9CI) (CA INDEX NAME)

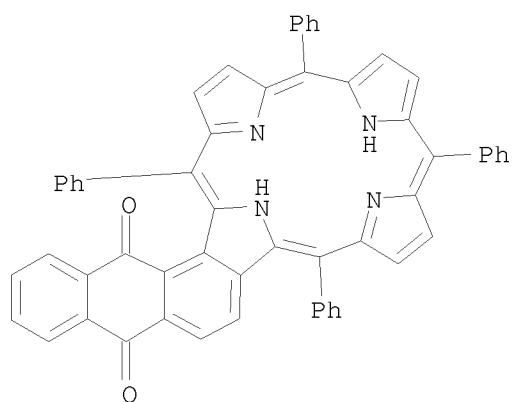
PAGE 1-A



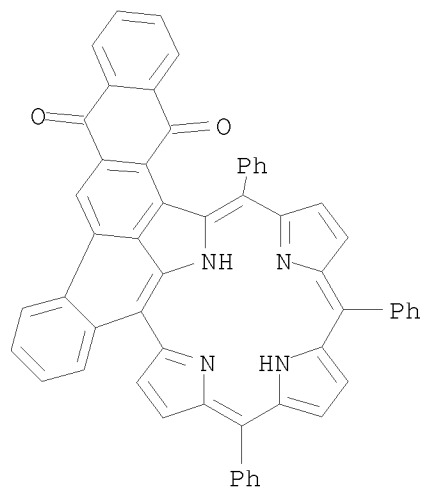
PAGE 2-A



IT 857254-10-5P 857254-11-6P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation by Diels-Alder reaction of nickel(II)  
 beta-vinyl-meso-tetraphenylporphyrin with naphthoquinone followed by  
 demetalation)  
 RN 857254-10-5 CAPLUS  
 CN 27H,29H-Anthra[1,2-b]porphine-21,26-dione, 2,7,12,17-tetraphenyl- (9CI)  
 (CA INDEX NAME)



RN 857254-11-6 CAPLUS  
 CN 17,19[1',2']-Benzeno-27H,29H-anthra[1,2-b]porphine-21,26-dione,  
 2,7,12-triphenyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 19 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:237611 CAPLUS

DOCUMENT NUMBER: 143:172462

TITLE: Instability of the molecular structure of monobenzoporphin to the alternation of the macrocycle bond lengths and its manifestation in the electronic spectra

AUTHOR(S): Kuz'mitskii, V. A.

CORPORATE SOURCE: Institute of Molecular and Atomic Physics, National Academy of Sciences of Belarus, Minsk, 220072, Belarus

SOURCE: Journal of Applied Spectroscopy (2004), 71(6), 777-787  
CODEN: JASYAP; ISSN: 0021-9037

PUBLISHER: Springer Science+Business Media, Inc.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Quantum-chemical calcns. of the geometric structure of the mols. of monobenzoporphin (H2 MBP) and monobenzoporphin with Me and Et substituents in the five-member rings (H2MBPm) were carried out by the restricted and UHF methods with the AM1 Hamiltonian (AM1 RHF and AM1 UHF methods). The calcn. of the above-indicated mols. by the AM1 RHF method without restrictions on their symmetry gave, for them, a planar structure with an alternation of the lengths of the bonds along the 18-member azacyclopolyene and the symmetry C<sub>1h</sub> for their aromatic part. The calcn. of the transitions to the excited electron Q states in such a structure by the CNDO/S method showed that these states are characterized by large hypsochromic shifts (.apprx.3000-4000 cm<sup>-1</sup>) relative to the Q levels of porphin (H2P), which is in contradiction with the exptl. data, according to which these shifts are bathochromic and comprise = -330 cm<sup>-1</sup> and = -750 cm<sup>-1</sup>. Optimization of the geometry of the H2 MBP and H2MBPm mols. by the AM1 UHF method gives, for them, a structure with equal lengths of the bonds along the 18-member azacyclopolyene with a symmetry differing insignificantly from the D<sub>2h</sub> symmetry; elements of the structure with a lower symmetry and an alternation of the lengths of the bonds are retained in the condensed pyrroline and benzene rings. The calcn. of the shifts of the Q levels in the H2MBPm mol. of this geometry relative to the analogous levels in H2P showed that they are bathochromic and equal to = -520 cm<sup>-1</sup>, and the RHF calcn. with optimization of the geometry of the mol. and restrictions on the effective symmetry D<sub>2h</sub> of the 18-member azacyclopolyene gave = -350 cm<sup>-1</sup> and = -430 cm<sup>-1</sup>. The restrictions imposed on the C<sub>2v</sub> symmetry of the H2MBP mols. by the RHF method are inadequate to equalize the lengths of the bonds along the 18-member azacyclopolyene. The calcns. of the energy of the B levels of the monobenzoporphyrins considered also lend credence to their geometric structure with equal lengths of the bonds along the 18-member azacyclopolyene.

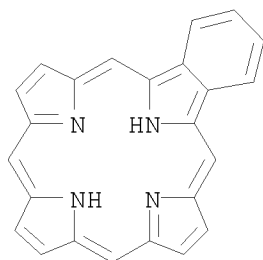
IT 36469-17-7, 23H,25H-Benzo[b]porphine 93614-17-6

RL: PRP (Properties)

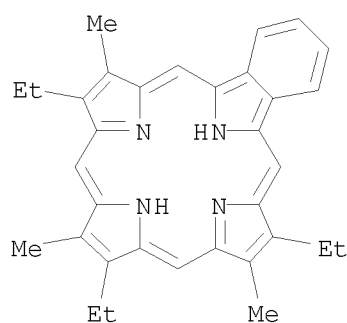
(instability of mol. structure of monobenzoporphine to related to alternation of macrocycle bond lengths and manifestation in UV spectra)

RN 36469-17-7 CAPLUS

CN 23H,25H-Benzo[b]porphine (9CI) (CA INDEX NAME)



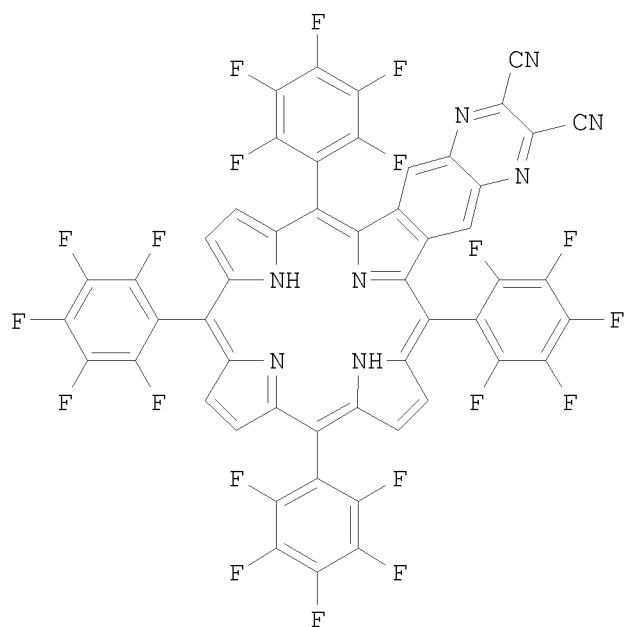
RN 93614-17-6 CAPLUS  
 CN 23H,25H-Benzo[b]porphine, 8,13,18-triethyl-9,14,19-trimethyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 20 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2005:199392 CAPLUS  
 DOCUMENT NUMBER: 142:430046  
 TITLE: Reaction of meso-tetraarylporphyrins with pyrazine ortho-quinodimethanes  
 AUTHOR(S): Zhao, Shengxian; Neves, Maria G. P. M. S.; Tome, Augusto C.; Silva, Artur M. S.; Cavaleiro, Jose A. S.; Domingues, Maria R. M.; Ferrer Correia, A. J.  
 CORPORATE SOURCE: Department of Chemistry, University of Aveiro, Aveiro, 3810-193, Port.  
 SOURCE: Tetrahedron Letters (2005), 46(13), 2189-2191  
 CODEN: TELEAY; ISSN: 0040-4039  
 PUBLISHER: Elsevier B.V.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 142:430046  
 GI





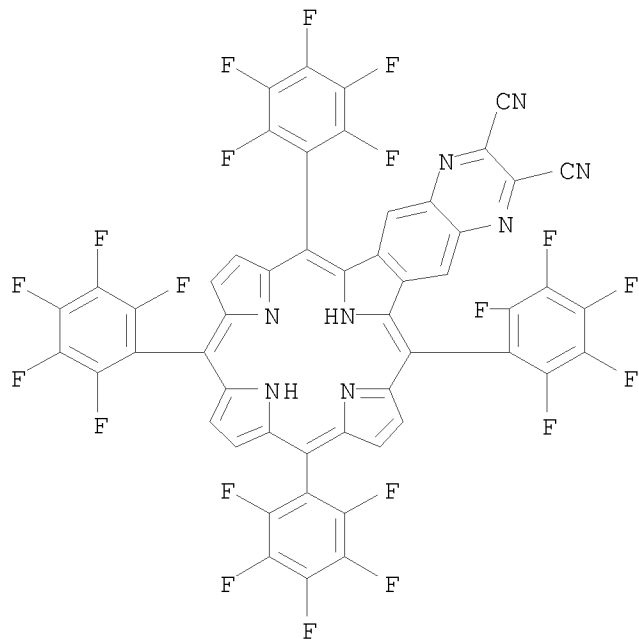
AB Novel  $\pi$ -extended porphyrins, e.g. I, were obtained from the Diels-Alder reaction of meso-tetraarylporphyrins with a pyrazine o-quinodimethane derivative

IT 850668-27-8P 850668-28-9P 850668-29-0P  
850668-30-3P 850668-31-4P 850668-32-5P  
850668-33-6P 850668-34-7P 850668-35-8P  
850668-36-9P 850668-37-0P 850668-38-1P

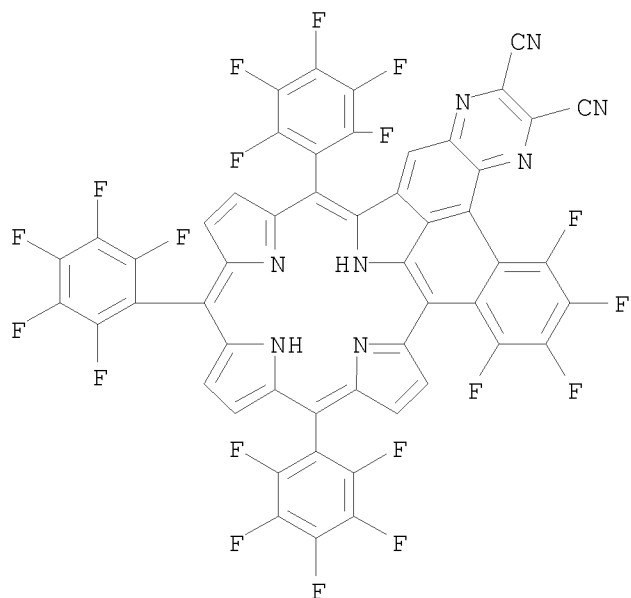
RL: SPN (Synthetic preparation); PREP (Preparation)  
(reaction of meso-tetraarylporphyrins with pyrazine  
ortho-quinodimethanes)

RN 850668-27-8 CAPLUS

CN 25H,27H-Quinoxalino[6,7-b]porphine-2,3-dicarbonitrile,  
7,12,17,22-tetrakis(pentafluorophenyl)- (9CI) (CA INDEX NAME)

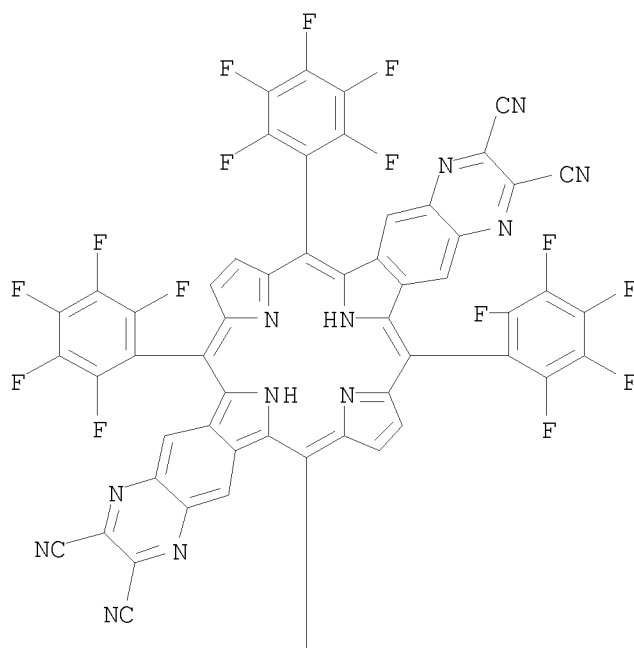


RN 850668-28-9 CAPLUS  
 CN 5,7[1',2']-Benzeno-25H,27H-quinoxalino[6,7-b]porphine-2,3-dicarbonitrile,  
 31,32,33,34-tetrafluoro-12,17,22-tris(pentafluorophenyl)- (9CI) (CA INDEX  
 NAME)

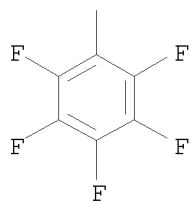


RN 850668-29-0 CAPLUS  
 CN 29H,31H-Diquinoxalino[6,7-b:6',7'-l]porphine-2,3,16,17-tetracarbonitrile,  
 7,12,21,26-tetrakis(pentafluorophenyl)- (9CI) (CA INDEX NAME)

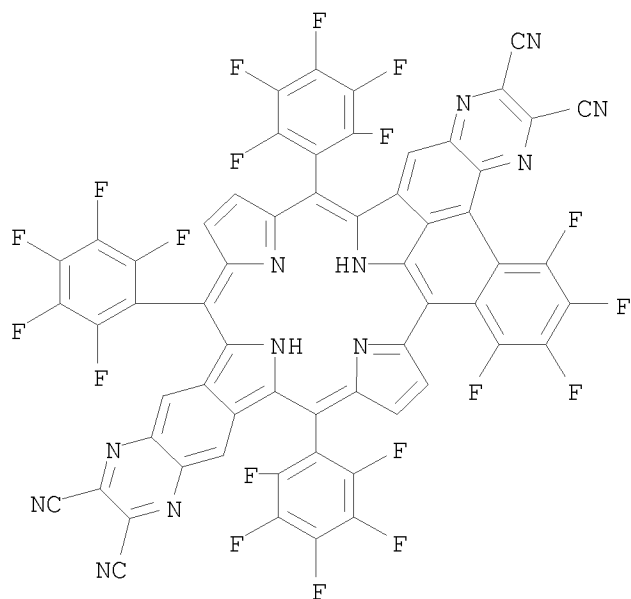
PAGE 1-A



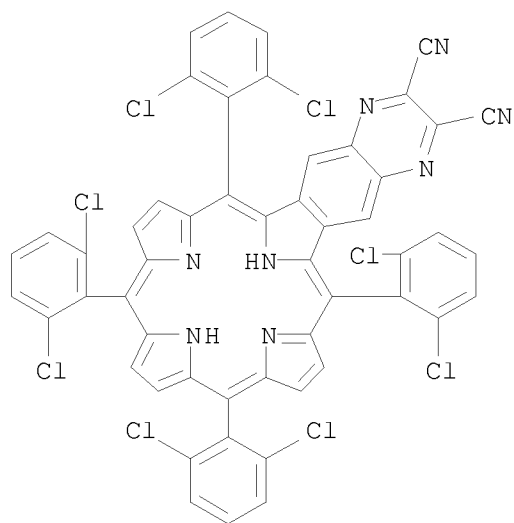
PAGE 2-A



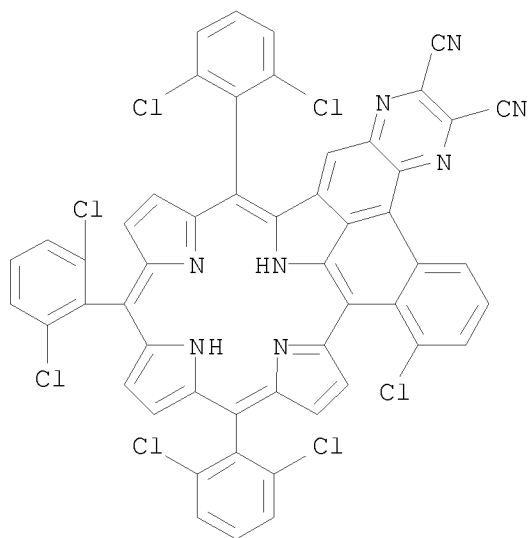
RN 850668-30-3 CAPLUS  
 CN 5,7[1',2']-Benzeno-29H,31H-diquinoxalino[6,7-b:6',7'-l]porphine-2,3,16,17-tetracarbonitrile, 35,36,37,38-tetrafluoro-12,21,26-tris(pentafluorophenyl)- (9CI) (CA INDEX NAME)



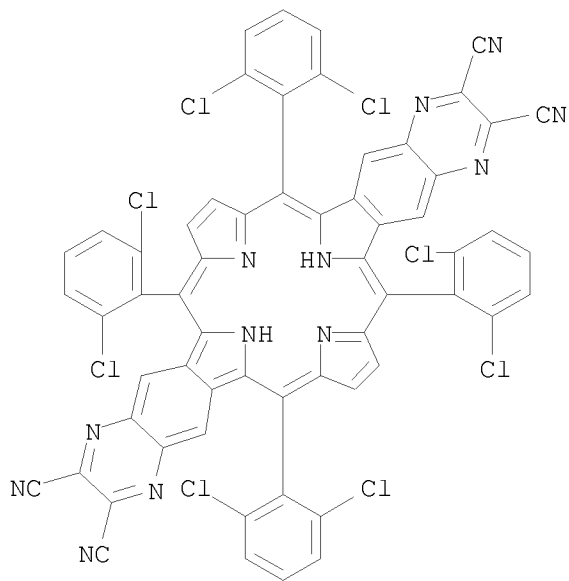
RN 850668-31-4 CAPLUS  
 CN 25H,27H-Quinoxalino[6,7-b]porphine-2,3-dicarbonitrile,  
 7,12,17,22-tetrakis(2,6-dichlorophenyl)- (9CI) (CA INDEX NAME)



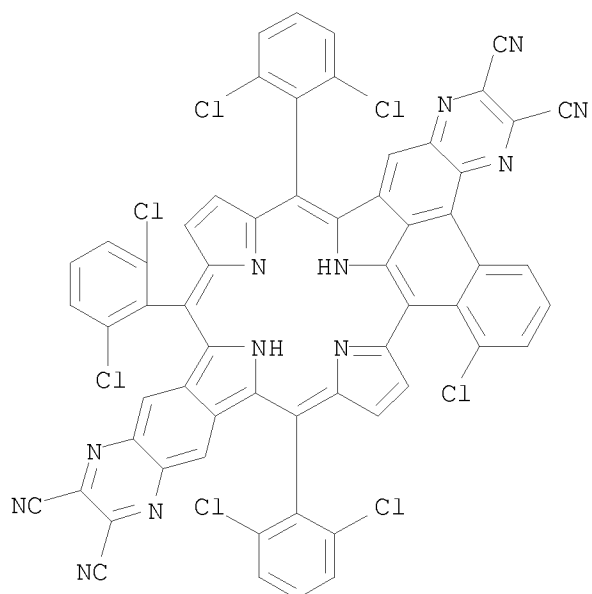
RN 850668-32-5 CAPLUS  
 CN 5,7[1',2']-Benzeno-25H,27H-quinoxalino[6,7-b]porphine-2,3-dicarbonitrile,  
 34-chloro-12,17,22-tris(2,6-dichlorophenyl)- (9CI) (CA INDEX NAME)



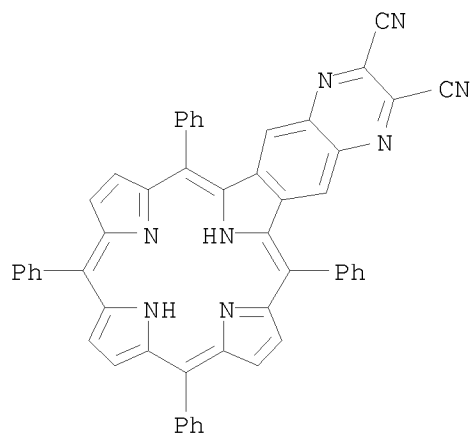
RN 850668-33-6 CAPLUS  
 CN 29H,31H-Diquinoxalino[6,7-b:6',7'-l]porphine-2,3,16,17-tetracarbonitrile,  
 7,12,21,26-tetrakis(2,6-dichlorophenyl)- (9CI) (CA INDEX NAME)



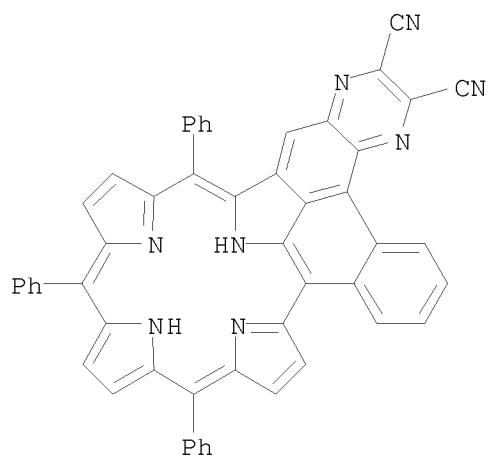
RN 850668-34-7 CAPLUS  
 CN 5,7[1',2']-Benzeno-29H,31H-diquinoxalino[6,7-b:6',7'-l]porphine-2,3,16,17-  
 tetracarbonitrile, 38-chloro-12,21,26-tris(2,6-dichlorophenyl)- (9CI) (CA  
 INDEX NAME)



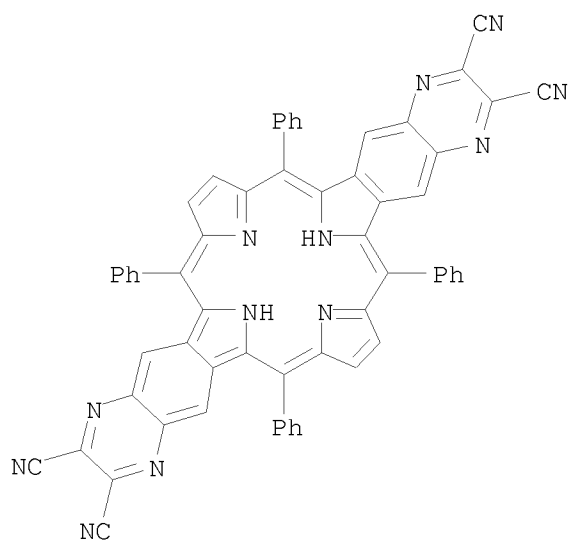
RN 850668-35-8 CAPLUS  
 CN 25H,27H-Quinoxalino[6,7-b]porphine-2,3-dicarbonitrile,  
 7,12,17,22-tetraphenyl- (9CI) (CA INDEX NAME)



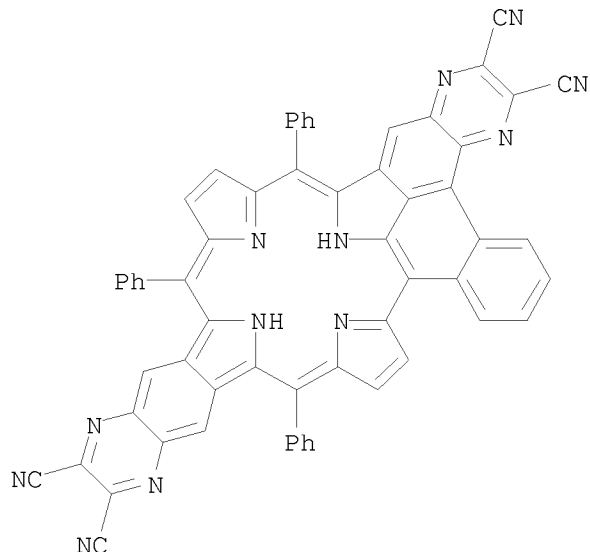
RN 850668-36-9 CAPLUS  
 CN 5,7[1',2']-Benzeno-25H,27H-quinoxalino[6,7-b]porphine-2,3-dicarbonitrile,  
 12,17,22-triphenyl- (9CI) (CA INDEX NAME)



RN 850668-37-0 CAPLUS  
 CN 29H,31H-Diquinoxalino[6,7-b:6',7'-1]porphine-2,3,16,17-tetracarbonitrile,  
 7,12,21,26-tetraphenyl- (9CI) (CA INDEX NAME)



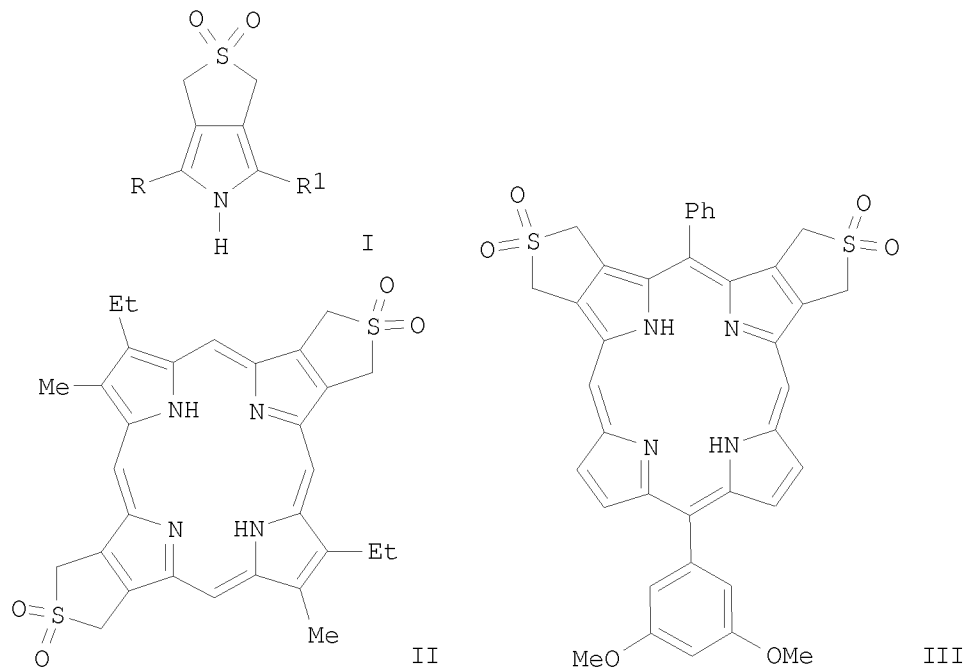
RN 850668-38-1 CAPLUS  
 CN 5,7[1',2']-Benzeno-29H,31H-diquinoxalino[6,7-b:6',7'-1]porphine-2,3,16,17-  
 tetracarbonitrile, 12,21,26-triphenyl- (9CI) (CA INDEX NAME)



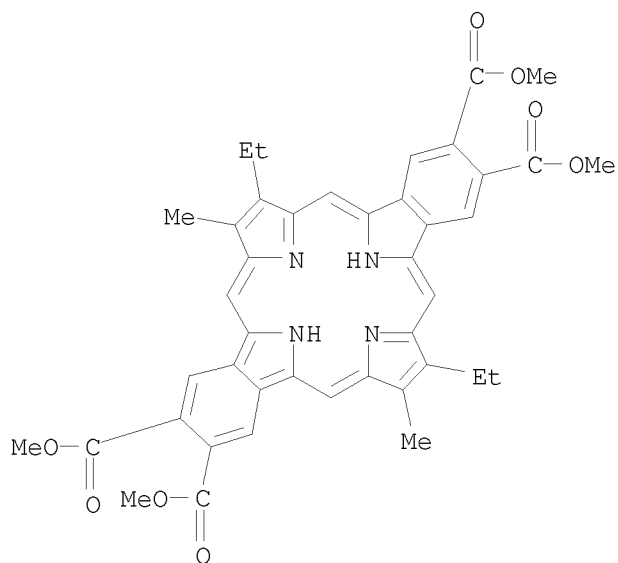
REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 21 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2005:169407 CAPLUS  
 DOCUMENT NUMBER: 142:411126  
 TITLE: Sulfolenoporphyrins: synthons for refunctionalization of porphyrins  
 AUTHOR(S): Lee, Sang Hee; Smith, Kevin M.  
 CORPORATE SOURCE: Department of Chemistry, Louisiana State University, Baton Rouge, LA, 70803, USA  
 SOURCE: Tetrahedron Letters (2005), 46(12), 2009-2013  
 CODEN: TELEAY; ISSN: 0040-4039  
 PUBLISHER: Elsevier B.V.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 142:411126  
 GI

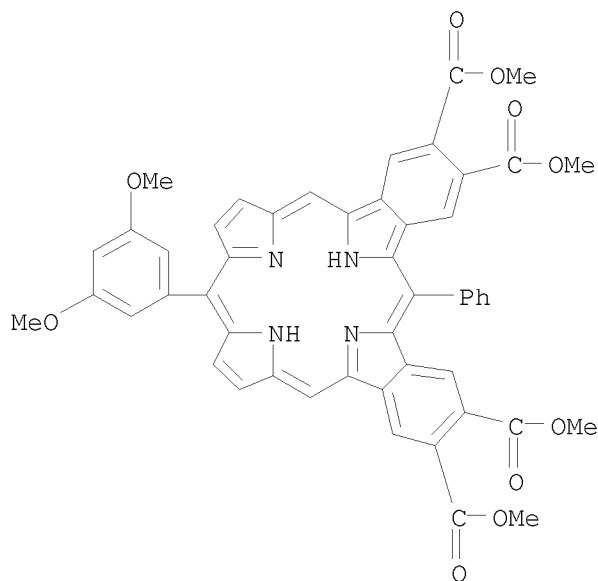




- AB Using sulfolenopyrroles I (R = H, R<sub>1</sub> = CO<sub>2</sub>CH<sub>2</sub>Ph) and I (R, R<sub>1</sub> = CHO), methods are developed for the synthesis of opp- (e.g II) and adj- (III) bis-sulfolenoporphyrins. Such compds. are useful building blocks for the refunctionalization of the porphyrin system, and readily undergo Diels-Alder cycloaddn. reactions.
- IT 850424-52-1P 850424-54-3P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of sulfolenoporphyrins as synthons for refunctionalization of porphyrins)
- RN 850424-52-1 CAPLUS
- CN 25H,27H-Dibenzo[b,1]porphine-2,3,14,15-tetracarboxylic acid,  
 8,21-diethyl-9,20-dimethyl-, tetramethyl ester (9CI) (CA INDEX NAME)



RN 850424-54-3 CAPLUS  
 CN 25H,27H-Dibenzo[b,g]porphine-2,3,19,20-tetracarboxylic acid,  
 13-(3,5-dimethoxyphenyl)-23-phenyl-, tetramethyl ester (9CI) (CA INDEX  
 NAME)



REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 22 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2005:95693 CAPLUS  
 DOCUMENT NUMBER: 142:347481

TITLE: Unexpected intramolecular cyclization of  
2-(perfluoroalkyl)tetraarylporphyrin radicals:  
Approaches for the intramolecular cyclization of  
2-(perfluoroalkyl)tetraarylporphyrin radicals

AUTHOR(S): Zeng, Zhuo; Liu, Chao; Jin, Li-Mei; Guo, Can-Cheng;  
Chen, Qing-Yun

CORPORATE SOURCE: College of Chemistry and Chemical Engineering, Hunan  
University, Changsha, 410082, Peop. Rep. China

SOURCE: European Journal of Organic Chemistry (2005), (2),  
306-316  
CODEN: EJOCFK; ISSN: 1434-193X

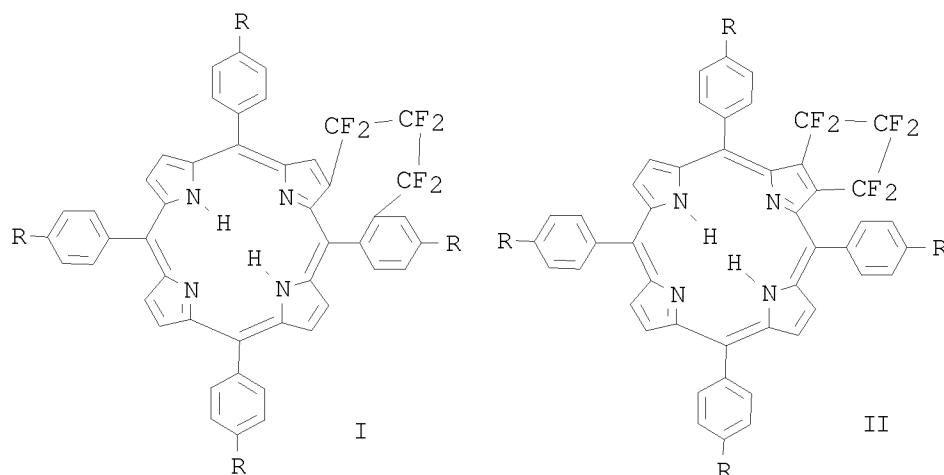
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 142:347481

GI



AB  $\beta$ -(Perfluoroalkyl)tetraarylporphyrin radicals, generated by the reaction of I(CF<sub>2</sub>)<sub>n</sub>X (n = 2-5; X = I, Cl) with porphyrins in the presence of Na<sub>2</sub>S<sub>2</sub>O<sub>4</sub>/NaHCO<sub>3</sub> in DMSO/CH<sub>2</sub>Cl<sub>2</sub> or DMSO, undergo cyclizations at the ortho position of a neighboring Ph ring and/or adjacent pyrrolic unit to give five-, six-, seven-, and eight-membered fused porphyrins, e.g., 5,10.15-triaryl[2-benzohexafluoro(21,22,23)]cyclooctanoporphyrins I and 5,10.15,20-tetraaryl-2-hexafluorocyclopentenylporphyrins II (R = H, Cl, Me for both). Porphyrins I and II could be separated as their zinc complexes, then demetalated. Crystal structures of I (R = H), the zinc(II) derivative of II (R = H), and of a tetrafluorobenzo analog of the latter zinc complex were determined

IT 848394-57-0P  
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(preparation and crystal structure of)

RN 848394-57-0 CAPLUS

CN Zinc, [1,2,3,4-tetrafluoro-6,11,16,21-tetraphenyl-23H,25H-benzo[b]porphinato(2-)-κN23,κN24,κN25,κN26]-,

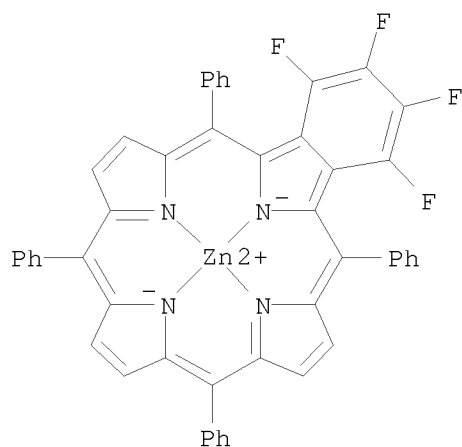
(SP-4-1)-, compd. with dichloromethane (1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 848394-49-0

CMF C48 H26 F4 N4 Zn

CCI CCS



CM 2

CRN 75-09-2

CMF C H2 Cl2

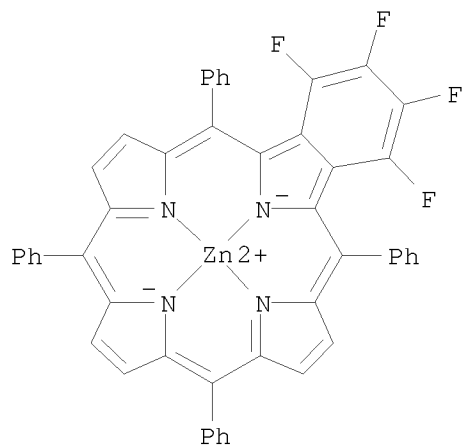
Cl-CH<sub>2</sub>-Cl

IT 848394-49-0P 848394-50-3P

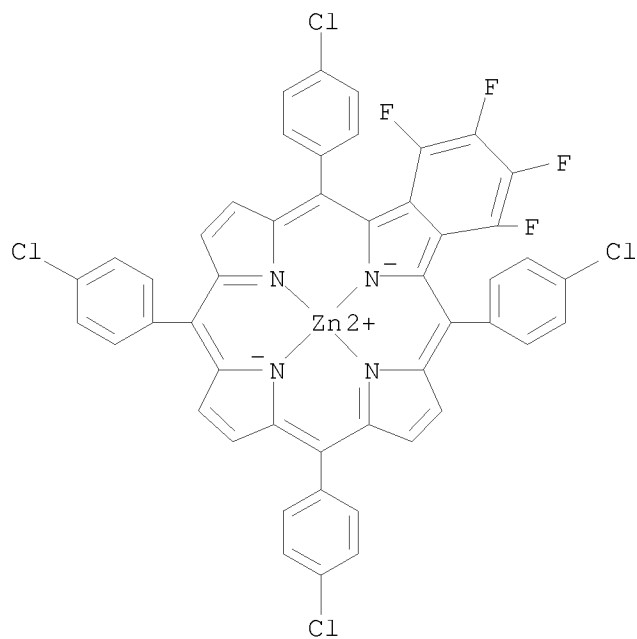
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and demetalation of)

RN 848394-49-0 CAPLUS

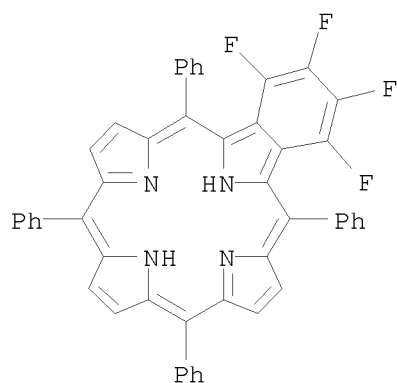
CN Zinc, [1,2,3,4-tetrafluoro-6,11,16,21-tetraphenyl-23H,25H-benzo[b]porphinato(2-)-κN23,κN24,κN25,κN26]-, (SP-4-1)- (CA INDEX NAME)



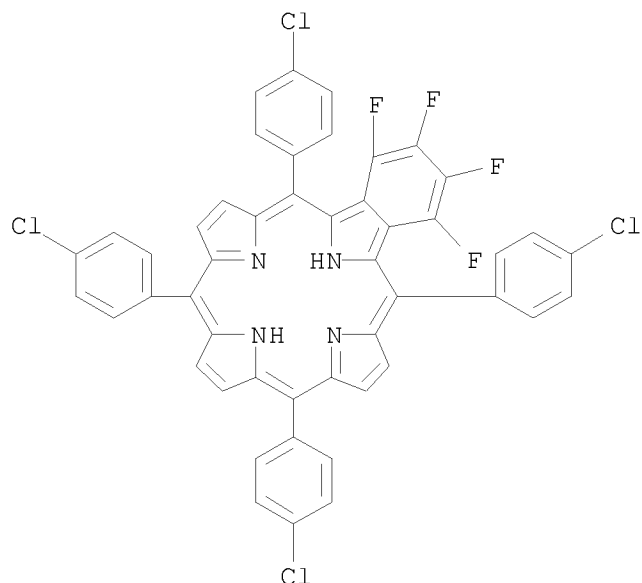
RN 848394-50-3 CAPLUS  
 CN Zinc, [6,11,16,21-tetrakis(4-chlorophenyl)-1,2,3,4-tetrafluoro-23H,25H-benzo[b]porphinato(2-)-κN23,κN24,κN25,κN26]-, (SP-4-1)- (9CI) (CA INDEX NAME)



IT 848394-52-5P 848394-53-6P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 RN 848394-52-5 CAPLUS  
 CN 23H,25H-Benzo[b]porphine, 1,2,3,4-tetrafluoro-6,11,16,21-tetraphenyl- (CA INDEX NAME)



RN 848394-53-6 CAPLUS  
 CN 23H,25H-Benzo[b]porphine, 6,11,16,21-tetrakis(4-chlorophenyl)-1,2,3,4-tetrafluoro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 23 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2005:48617 CAPLUS  
 DOCUMENT NUMBER: 142:282431  
 TITLE: Characterization of Petroporphyrins Using Ultraviolet-Visible Spectroscopy and Laser Desorption Ionization Time-of-Flight Mass Spectrometry  
 AUTHOR(S): Xu, Hai; Que, Guohe; Yu, Daoyong; Lu, Jian R.  
 CORPORATE SOURCE: State Key Laboratory of Heavy Oil Processing, College of Chemistry and Chemical Engineering, University of Petroleum, Dongying, 257061, Peop. Rep. China  
 SOURCE: Energy & Fuels (2005), 19(2), 517-524  
 CODEN: ENFUEM; ISSN: 0887-0624

PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB Petroporphyrins were extracted from two typical Chinese heavy crude oils, Tahe and Du84, and then purified by silica gel chromatog., followed by demetallization by Me sulfonic acid. The extraction and purification were monitored

using UV-visible spectroscopy, and the final petroporphyrins were analyzed using laser desorption ionization time-of-flight mass spectrometry. The soft ionization mass spectrometric technique proved to be effective for the characterization of petroporphyrins. The results show that, in Tahe crude oil, vanadium is more abundant than nickel and 75% of the vanadyl porphyrins are of the etioporphyrin (ETIO) type, with remaining fractions attributed to deoxophylloerythroetioporphyrin (DPEP) and benzo types. The  $\Sigma\text{DPEP}/\Sigma\text{ETIO}$  ratio was found to be 0.18. In contrast, the Du84 heavy crude oil contains more abundant nickel than vanadium, with its nickel porphyrins comprising mainly DPEP and ETIO types, with each occupying 45%, and the tetrahydrobenzo-DPEP and benzo types attributed to the remaining 10%. The  $\Sigma\text{DPEP}/\Sigma\text{ETIO}$  ratio is .apprx.1.1. These results suggest that the Tahe crude oil has higher thermal maturity than the Du84 crude oil, and the former is in its mature stage, whereas the latter is in its evolution stage.

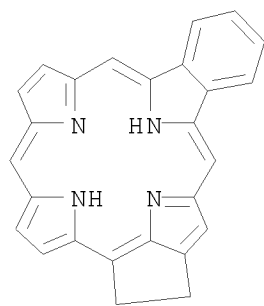
IT 128920-36-5D, derivs., vanadyl and nickel complexes  
 844635-65-0D, derivs., nickel complexes

RL: ANT (Analyte); OCU (Occurrence, unclassified); ANST (Analytical study); OCCU (Occurrence)

(characterization of petroporphyrins using UV-visible spectroscopy and laser desorption ionization time-of-flight mass spectrometry)

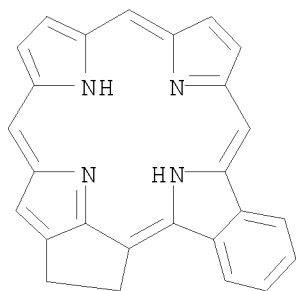
RN 128920-36-5 CAPLUS

CN 5,22:12,15-Diimino-20,18-metheno-7,10-nitrilobenzo[o]cyclopent[b]azacyclononadecine, 16,17-dihydro- (9CI) (CA INDEX NAME)



RN 844635-65-0 CAPLUS

CN 7,10:17,22-Diimino-5,3-metheno-12,15-nitrilobenzo[e]cyclopent[b]azacyclononadecine, 1,2-dihydro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 24 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2005:3712 CAPLUS  
 DOCUMENT NUMBER: 142:308595  
 TITLE: Synthesis of Isomeric Angularly Annealed Dinaphthoporphyryrin Systems: Examination of the Relative Positioning and Orientation of Ring Fusion as Factors Influencing the Porphyrin Chromophore  
 AUTHOR(S): Manley, Jerad M.; Roper, Tracy J.; Lash, Timothy D.  
 CORPORATE SOURCE: Department of Chemistry, Illinois State University, Normal, IL, 61790-4160, USA  
 SOURCE: Journal of Organic Chemistry (2005), 70(3), 874-891  
 CODEN: JOCEAH; ISSN: 0022-3263  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 142:308595  
 GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB Porphyrins built up from two naphtho[1,2-c]pyrrole subunits and two  $\beta$ -substituted pyrroles can produce five isomeric dinaphthoporphyryrin systems. To gain insights into the effects of ring fusion on extended porphyrin chromophores, all five of these systems, I-V derivs., were synthesized in isomerically pure form. In four of these syntheses, dihydronaphthopyrroles were used to introduce one or both of the naphthalene subunits, and dehydrogenation with DDQ in refluxing toluene later produced the fully conjugated systems. Naphthopyrroles were also prepared by reacting isocyanoacetate esters with 1-nitronaphthalene in the presence of a phosphazene base. These compds. proved to be less stable than their dihydronaphthopyrrolic counterparts, but could still be used in these synthetic studies. Three isomeric adj-dinaphthoporphyryrin systems were prepared using the MacDonald 2 + 2 condensation or by the cyclization of a,c-biladiene intermediates with CuCl<sub>2</sub> or AgIO<sub>3</sub>-Zn(OAc)<sub>2</sub>. A dinaphthoporphyryrin with two naphthalene units pointing toward one another could only be obtained in low yields due to a combination of stability and steric factors, but the other two adj-di-fused systems were isolated in good overall yields. However, the final dehydrogenation step occurred in



moderate yields (50-60%) and could only be performed when the porphyrins bore propionate ester side chains that produced sufficient solubility in organic

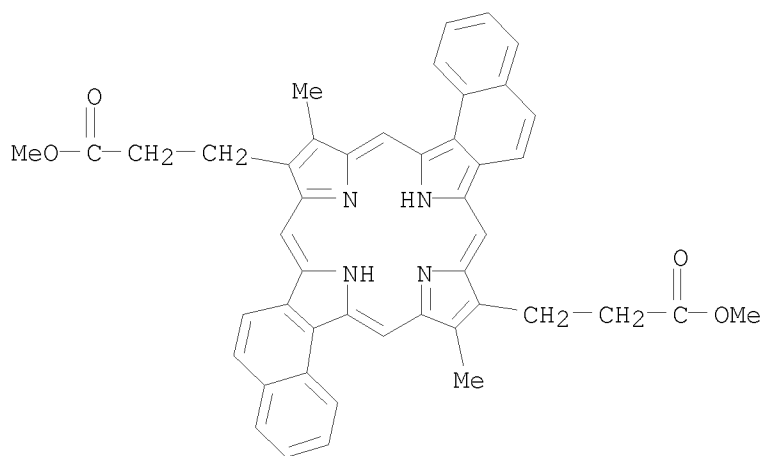
solvents. The two related opp-dinaphthoporphyrins were synthesized by a head-to-tail self-condensation of a dipyrromethane aldehyde, or a 3 + 1 synthesis using a tripyrrane intermediate bearing two fused dihydronaphthalene moieties, in excellent yields. In both cases, a final dehydrogenation step was required, but the opp-dinaphthoporphyrins were consistently formed in virtually quant. yields. The opp-dinaphthoporphyrin series gave UV-visible spectra with relatively strong Soret bands at 425 nm, and the visible region was dominated by an unusually strong Q-band III. The adj-dinaphthoporphyrins produced broader less intense Soret bands and four well-defined Q-bands, including a relatively strong absorption at 645 nm. However, the relative orientation of the naphthalene rings had no significant effects on these spectra. The dications produced in TFA-CHCl<sub>3</sub> solns. showed more discrimination between the individual porphyrin systems, and the metallo derivs. also displayed significant variations in their electronic absorption spectra.

IT 159469-67-7P 845784-90-9P 845784-91-0P  
845784-92-1P 845784-93-2P 845784-94-3P  
845784-95-4P 845785-00-4P 845785-01-5P  
845785-02-6P 845785-10-6P 845785-11-7P  
845785-12-8P 845785-18-4P 845785-19-5P  
845785-20-8P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(preparation and effect of ring fusion position/orientation on UV-visible of porphyrin chromophore)

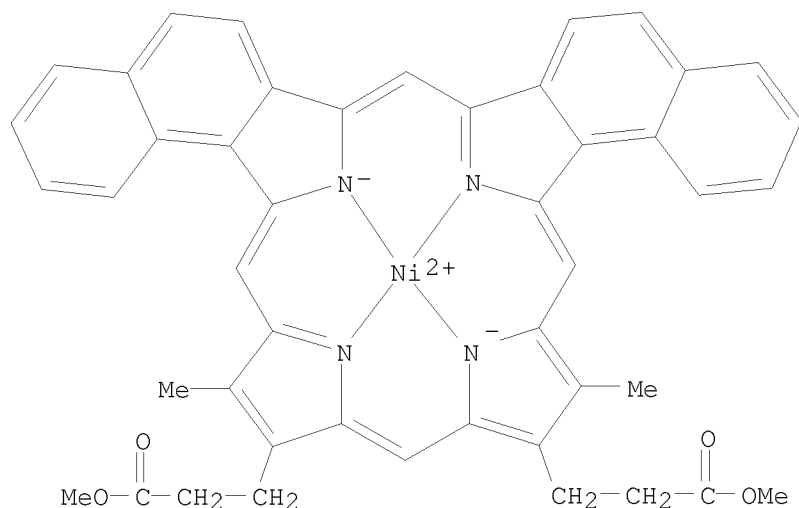
RN 159469-67-7 CAPLUS

CN 29H,31H-Dinaphtho[1,2-b:1',2'-l]porphine-10,24-dipropanoic acid,  
11,25-dimethyl-, dimethyl ester (9CI) (CA INDEX NAME)



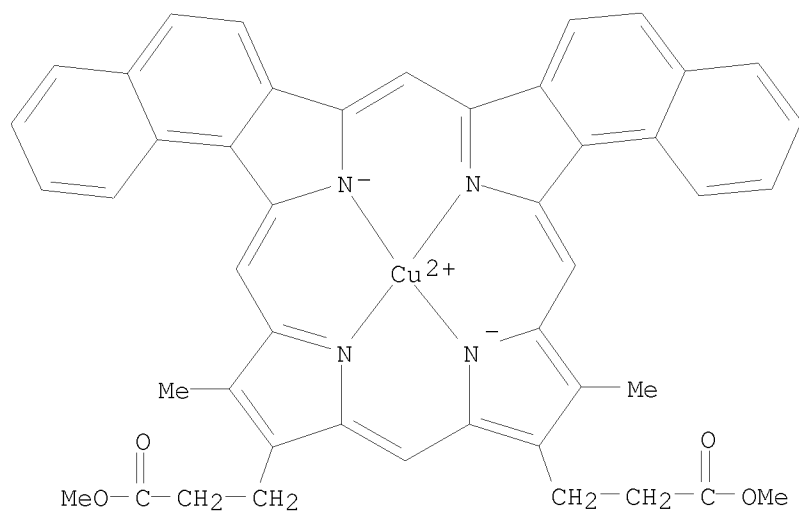
RN 845784-90-9 CAPLUS

CN Nickel, [dimethyl 19,25-dimethyl-29H,31H-dinaphtho[1,2-b:2',1'-g]porphine-20,24-dipropanoato(2-)-κN29,κN30,κN31,κN32]-, (SP-4-2)- (9CI) (CA INDEX NAME)



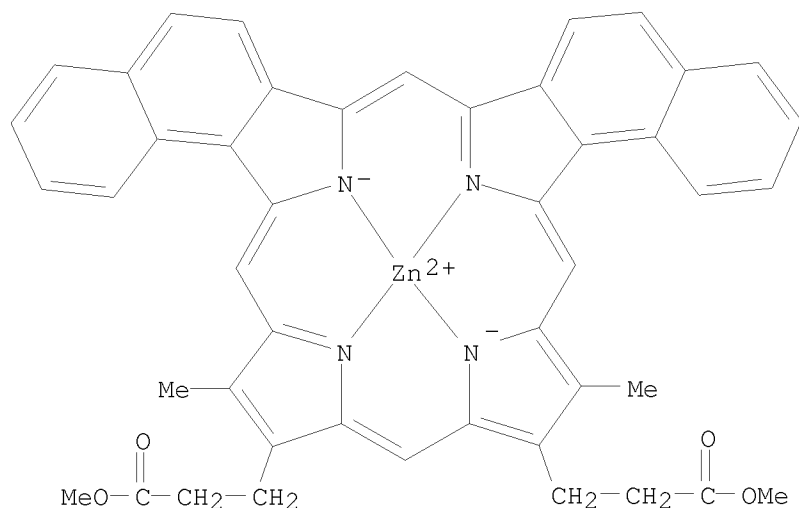
RN 845784-91-0 CAPLUS

CN Copper, [dimethyl 19,25-dimethyl-29H,31H-dinaphtho[1,2-b:2',1'-g]porphine-20,24-dipropanoato(2-)- $\kappa\text{N}29,\kappa\text{N}30,\kappa\text{N}31,\kappa\text{N}32$ ]-, (SP-4-2)- (9CI) (CA INDEX NAME)



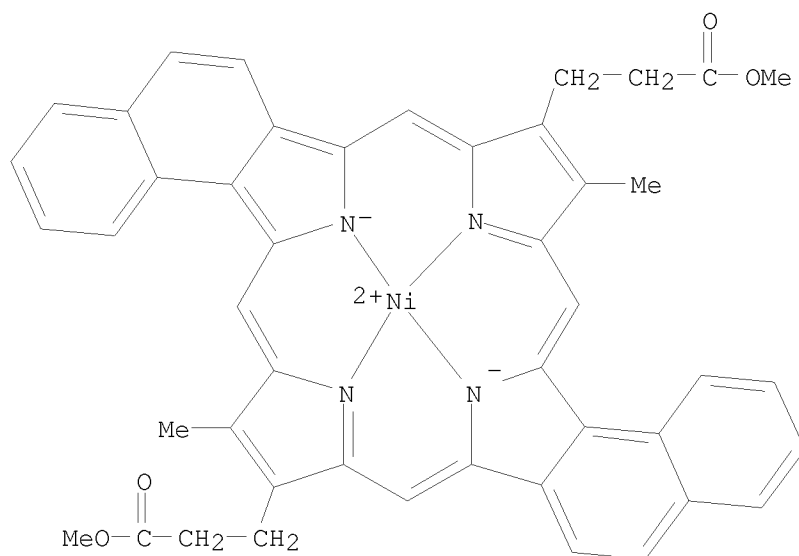
RN 845784-92-1 CAPLUS

CN Zinc, [dimethyl 19,25-dimethyl-29H,31H-dinaphtho[1,2-b:2',1'-g]porphine-20,24-dipropanoato(2-)- $\kappa\text{N}29,\kappa\text{N}30,\kappa\text{N}31,\kappa\text{N}32$ ]-, (SP-4-2)- (9CI) (CA INDEX NAME)



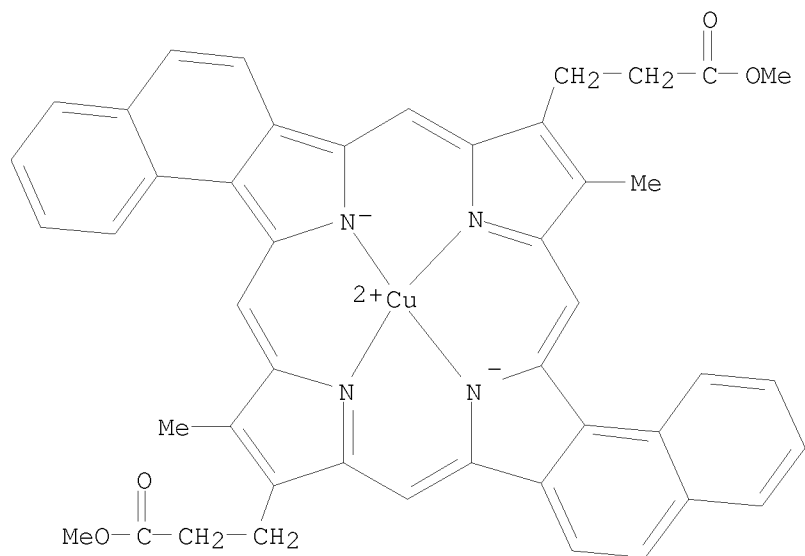
RN 845784-93-2 CAPLUS

CN Nickel, [dimethyl 11,25-dimethyl-29H,31H-dinaphtho[1,2-b:1',2'-1]porphine-10,24-dipropanoato(2-)- $\kappa\text{N}29,\kappa\text{N}30,\kappa\text{N}31,\kappa\text{N}32$ ]-, (SP-4-1)- (9CI) (CA INDEX NAME)

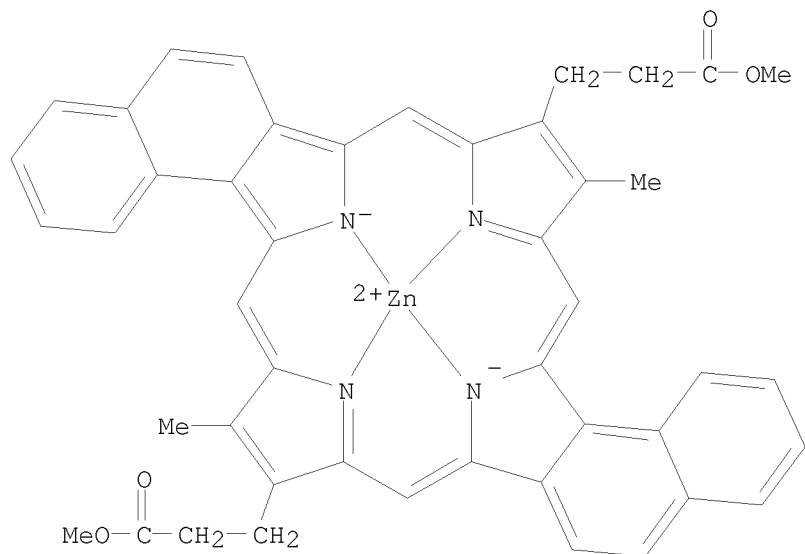


RN 845784-94-3 CAPLUS

CN Copper, [dimethyl 11,25-dimethyl-29H,31H-dinaphtho[1,2-b:1',2'-1]porphine-10,24-dipropanoato(2-)- $\kappa\text{N}29,\kappa\text{N}30,\kappa\text{N}31,\kappa\text{N}32$ ]-, (SP-4-1)- (9CI) (CA INDEX NAME)

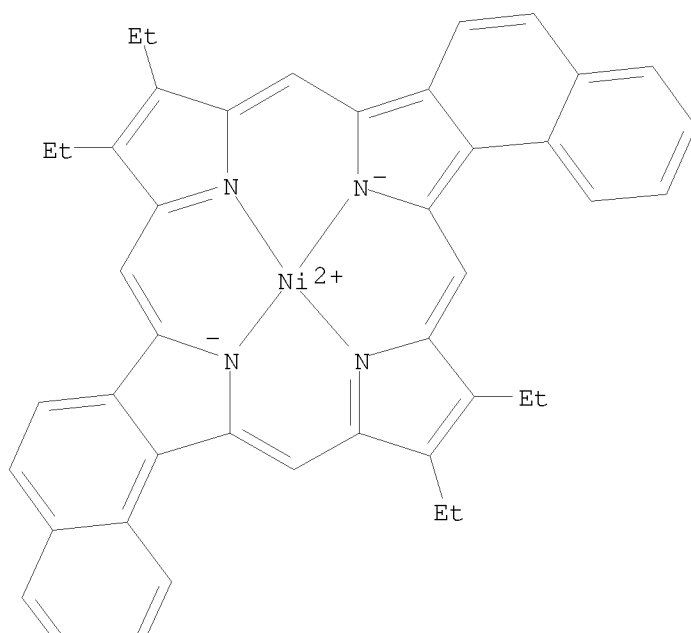


RN 845784-95-4 CAPLUS  
 CN Zinc, [dimethyl 11,25-dimethyl-29H,31H-dinaphtho[1,2-b:1',2'-l]porphine-10,24-dipropanoato(2-)-κN29,κN30,κN31,κN32]-, (SP-4-1)- (9CI) (CA INDEX NAME)



RN 845785-00-4 CAPLUS  
 CN Nickel, [10,11,24,25-tetraethyl-29H,31H-dinaphtho[1,2-b:1',2'-l]porphinato(2-)-κN29,κN30,κN31,κN32]-, (SP-4-2)- (9CI) (CA INDEX NAME)

PAGE 1-A

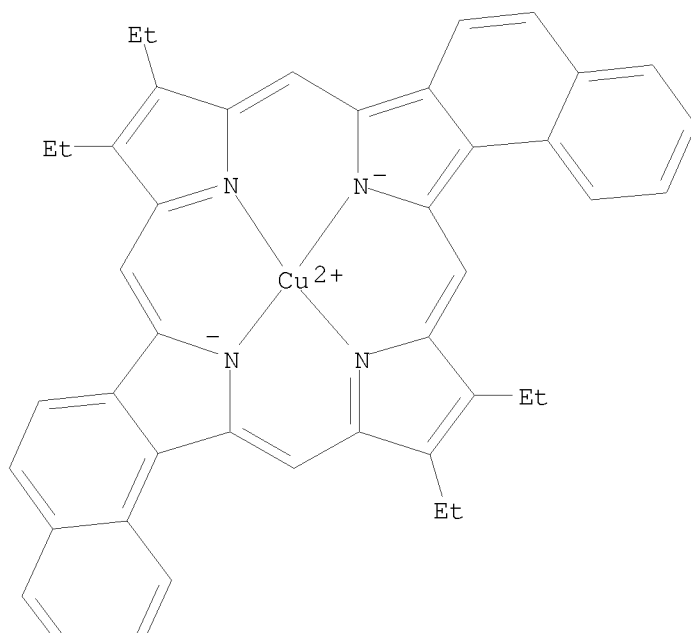


PAGE 2-A



RN 845785-01-5 CAPLUS  
 CN Copper, [10,11,24,25-tetraethyl-29H,31H-dinaphtho[1,2-b:1',2'-  
 1]porphinato(2-)-κN29,κN30,κN31,κN32]-, (SP-4-2)-  
 (9CI) (CA INDEX NAME)

PAGE 1-A

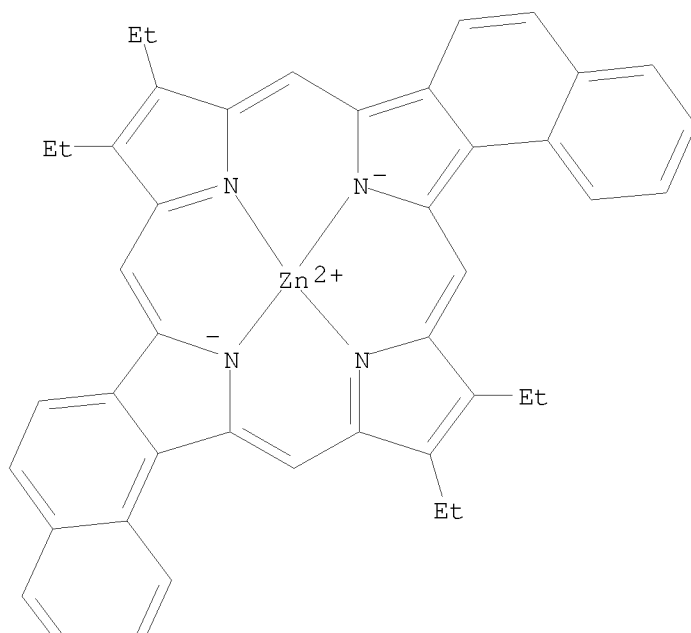


PAGE 2-A



RN 845785-02-6 CAPLUS  
 CN Zinc, [10,11,24,25-tetraethyl-29H,31H-dinaphtho[1,2-b:1',2'-1]porphinato(2-)-κN29,κN30,κN31,κN32]-, (SP-4-2)- (9CI) (CA INDEX NAME)

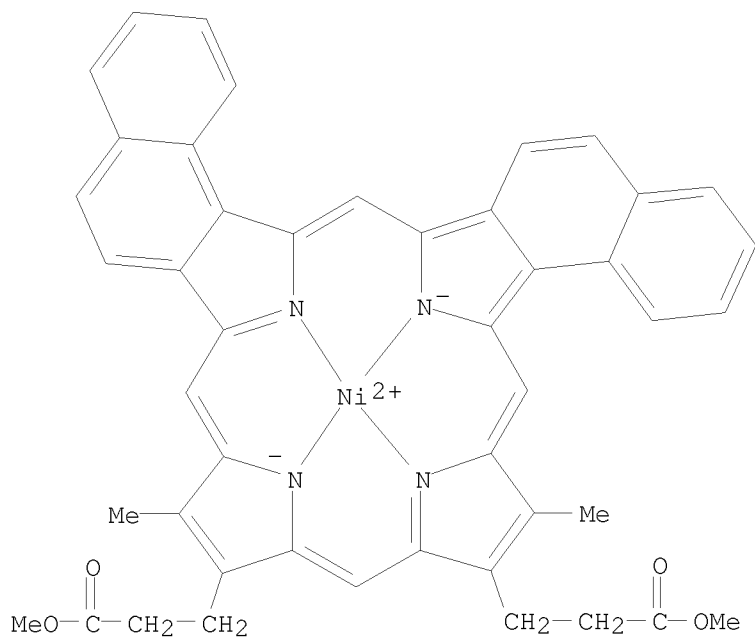
PAGE 1-A



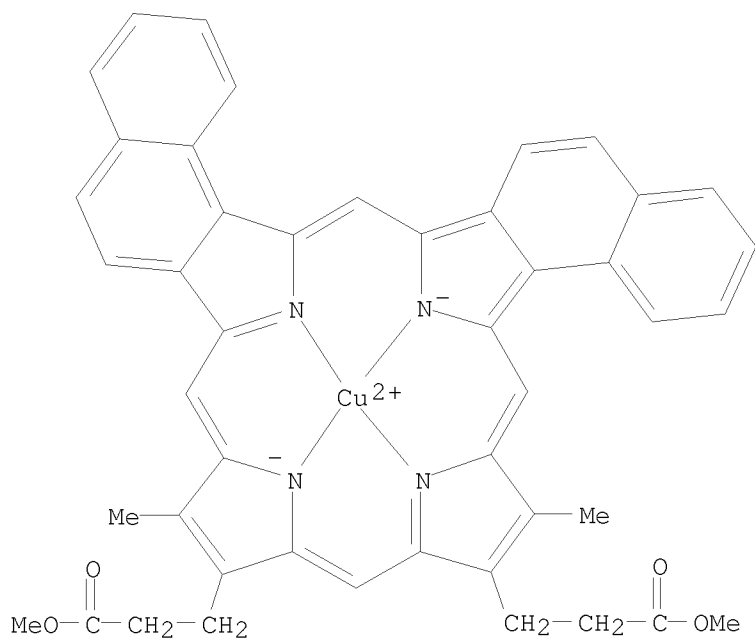
PAGE 2-A



RN 845785-10-6 CAPLUS  
 CN Nickel, [dimethyl 8,14-dimethyl-29H,31H-dinaphtho[1,2-b:1',2'-g]porphine-9,13-dipropionato(2-)-κN29,κN30,κN31,κN32]-, (SP-4-2)- (9CI) (CA INDEX NAME)



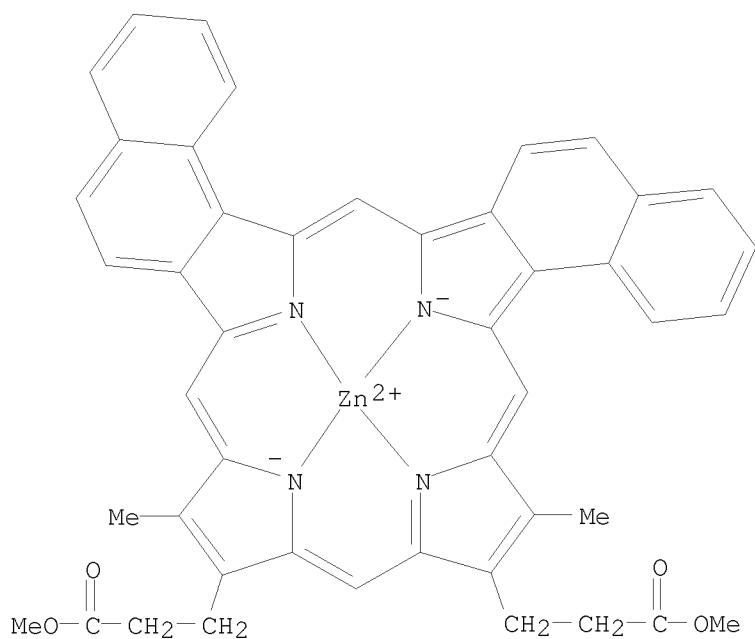
RN 845785-11-7 CAPLUS  
 CN Copper, [dimethyl 8,14-dimethyl-29H,31H-dinaphtho[1,2-b:1',2'-g]porphine-9,13-dipropanoato(2-)- $\kappa\text{N}29,\kappa\text{N}30,\kappa\text{N}31,\kappa\text{N}32$ ]-, (SP-4-2)- (9CI) (CA INDEX NAME)



RN 845785-12-8 CAPLUS  
 CN Zinc, [dimethyl 8,14-dimethyl-29H,31H-dinaphtho[1,2-b:1',2'-g]porphine-

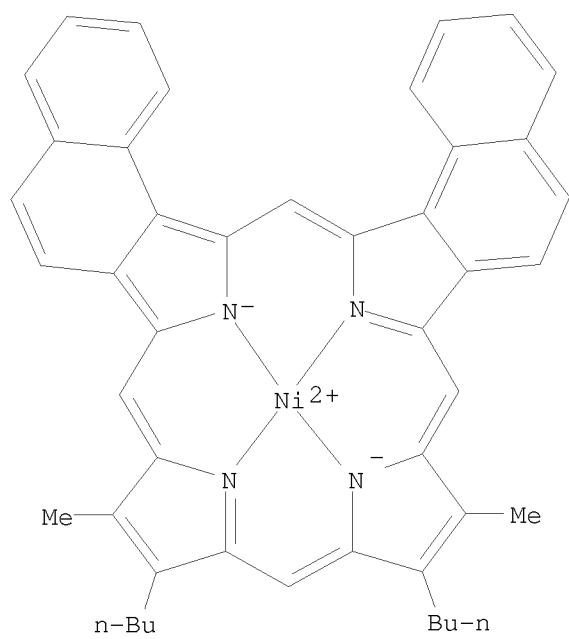


9,13-dipropanoato(2-)- $\kappa$ N29, $\kappa$ N30, $\kappa$ N31, $\kappa$ N32]-,  
(SP-4-2)- (9CI) (CA INDEX NAME)



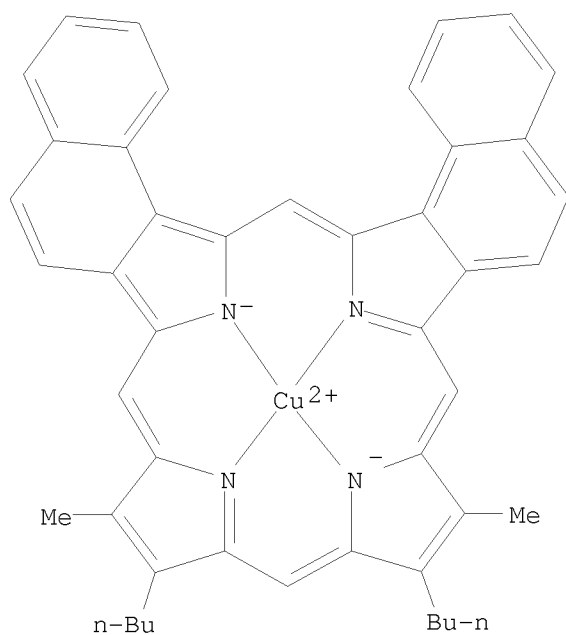
RN 845785-18-4 CAPLUS

CN Nickel, [11,15-dibutyl-10,16-dimethyl-29H,31H-dinaphtho[2,1-b:1',2'-g]porphinato(2-)- $\kappa$ N29, $\kappa$ N30, $\kappa$ N31, $\kappa$ N32]-, (SP-4-2)-  
(9CI) (CA INDEX NAME)



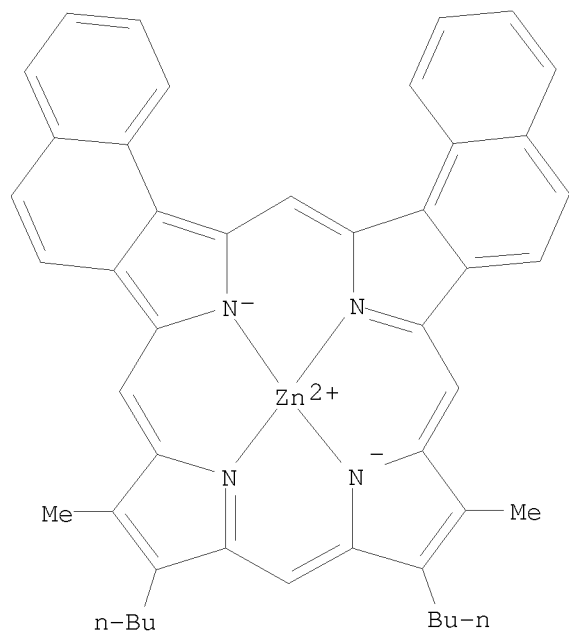
RN 845785-19-5 CAPLUS

CN Copper, [11,15-dibutyl-10,16-dimethyl-29H,31H-dinaphtho[2,1-b:1',2'-g]porphinato(2-)-κN29,κN30,κN31,κN32]-, (SP-4-2)-(9CI) (CA INDEX NAME)

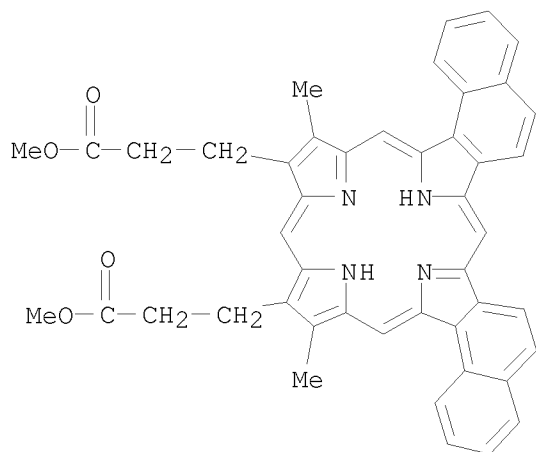


RN 845785-20-8 CAPLUS

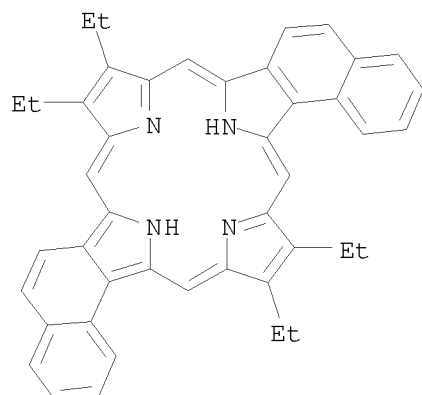
CN Zinc, [11,15-dibutyl-10,16-dimethyl-29H,31H-dinaphtho[2,1-b:1',2'-g]porphinato(2-)-κN29,κN30,κN31,κN32]-, (SP-4-2)-(9CI) (CA INDEX NAME)



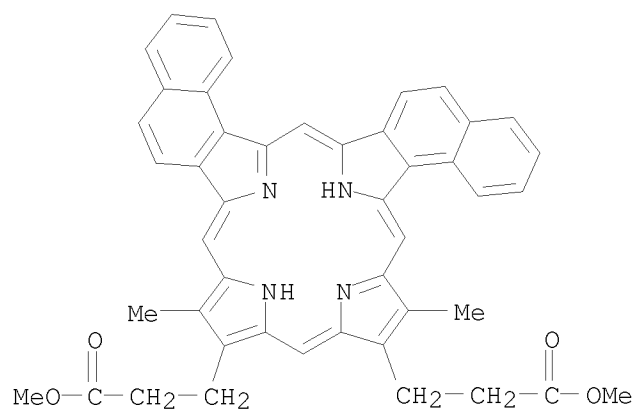
IT 159469-60-0P 845784-99-8P 845785-09-3P  
 845785-14-0P  
 RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP  
 (Preparation); RACT (Reactant or reagent)  
 (preparation, metalation, and effect of ring fusion position/orientation on  
 UV-visible of porphyrin chromophore)  
 RN 159469-60-0 CAPLUS  
 CN 29H,31H-Dinaphtho[1,2-b:2',1'-g]porphine-20,24-dipropanoic acid,  
 19,25-dimethyl-, dimethyl ester (9CI) (CA INDEX NAME)



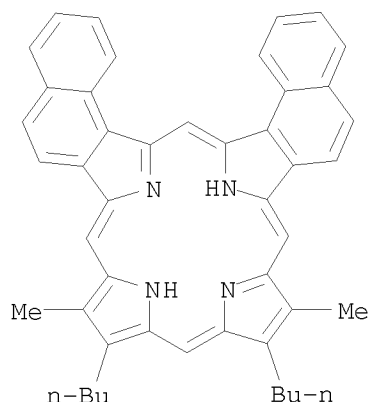
RN 845784-99-8 CAPLUS  
 CN 29H,31H-Dinaphtho[1,2-b:2',1'-l]porphine, 10,11,24,25-tetraethyl- (9CI)  
 (CA INDEX NAME)



RN 845785-09-3 CAPLUS  
 CN 29H,31H-Dinaphtho[1,2-b:1',2'-g]porphine-9,11-dipropenoic acid,  
 8,14-dimethyl-, dimethyl ester (9CI) (CA INDEX NAME)



RN 845785-14-0 CAPLUS  
 CN 29H,31H-Dinaphtho[2,1-b:1',2'-g]porphine, 11,13-dibutyl-10,15-dimethyl-  
 (9CI) (CA INDEX NAME)



REFERENCE COUNT: 102 THERE ARE 102 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 25 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:1106815 CAPLUS

DOCUMENT NUMBER: 142:231810

TITLE: Controlling Both Ground- and Excited-State Thermal Barriers to Bergman Cyclization with Alkyne Termini Substitution

AUTHOR(S): Nath, Mahendra; Pink, Maren; Zaleski, Jeffrey M.

CORPORATE SOURCE: Department of Chemistry, Indiana University, Bloomington, IN, 47405, USA

SOURCE: Journal of the American Chemical Society (2005), 127(2), 478-479

CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

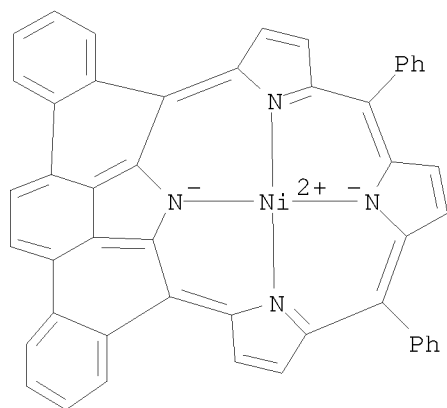
LANGUAGE: English

OTHER SOURCE(S): CASREACT 142:231810

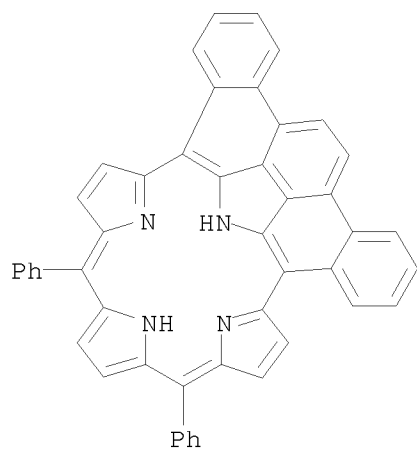
AB The cross-coupling reaction of 2,3-dibromo-5,10,15,20-tetraphenylporphyrin with corresponding organostannanes in the presence of a Pd0 catalyst in THF at reflux temperature yields free base 2,3-dialkynylporphyrins 1a,c-e. The subsequent deprotection of trimethylsilyl group of 1a with TBAF in THF under aqueous conditions produces the 2,3-diethynyl-5,10,15,20-tetraphenylporphyrin 1b in 87% yield. Compds. 1a-d undergo Zn insertion upon treatment with Zn(OAc)2·2H2O in CHCl3/MeOH to give Zn(II) 2,3-dialkynyl-5,10,15,20-tetraphenylporphyrins (2a-d) in 70-92% yields. Thermal Bergman cyclization of 1a-e and 2a-d was studied in chlorobenzene and .apprx.35-fold 1,4-cyclohexadiene at 120-210°. 1B and 2b (R = H) react at lower temperature (120°) and produce cyclized products 3b and 4b in higher yields (65-70%) than their Pr, iso-Pr, and Ph analogs, with R = Ph being the most stable. Continuing in this trend, the -TMS derivs. 1a and 2a exhibit no reactivity even after heating at 190° in chlorobenzene/cyclohexadiene for 24 h. Photolysis (at  $\lambda \geq 395$  nm) of 1b and 2b at 10° leads the formation of isolable picenoporphyrin products in 15 and 35% yields, resp., in 72 h, whereas these compds. are stable in solution under same reaction conditions at 25° in the dark. Unlike thermolysis at 125°, which did not yield Bergman cyclized product for R = Ph, photolysis generated very small

amts. of picenoporphyrin products (3c: 5%; 4c: 8% based on  $^1\text{H}$  NMR) as well as a mixture of reduced porphyrin products that were not separable. Thus, trends in the barrier to Bergman cyclization in the excited state exhibit the same trend as those observed in the ground state as a function of R-group. Finally, photolysis of 2b at  $10^\circ$  with  $\lambda \geq 515$  or  $590$  nm in benzene/iPrOH (4:1, 72 h) produces 4b in 15 and 6% isolated yields, indicating that conjugation of the enediyne unit into the porphyrin electronic transitions leads to sufficient distortion to generate photoproduct even with long wavelength excitation.

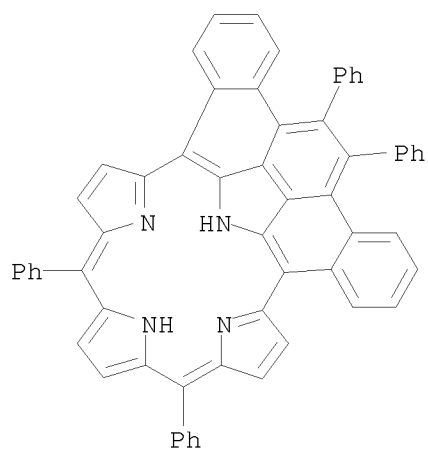
IT 380447-58-5P  
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
 (preparation and crystal structure)  
 RN 380447-58-5 CAPLUS  
 CN Nickel, [11,16-diphenyl-1,21[1',2']:4,6[1'',2'']-dibenzeno-23H,25H-benzo[b]porphinato(2-)- $\kappa\text{N}23,\kappa\text{N}24,\kappa\text{N}25,\kappa\text{N}26$ ]-, (SP-4-1)-(9CI) (CA INDEX NAME)



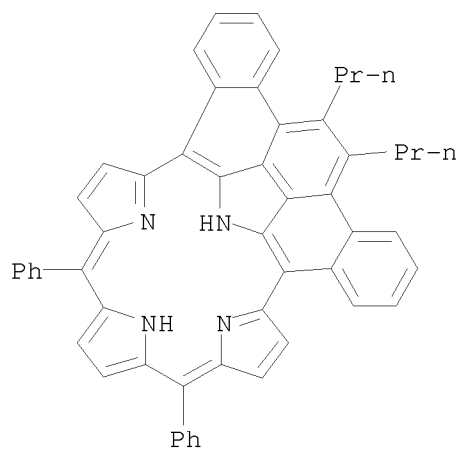
IT 564475-27-0P 842125-59-1P 842125-60-4P  
 842125-61-5P 842125-62-6P 842125-63-7P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 RN 564475-27-0 CAPLUS  
 CN 1,21[1',2']:4,6[1'',2'']-Dibenzeno-23H,25H-benzo[b]porphine,  
 11,16-diphenyl- (9CI) (CA INDEX NAME)



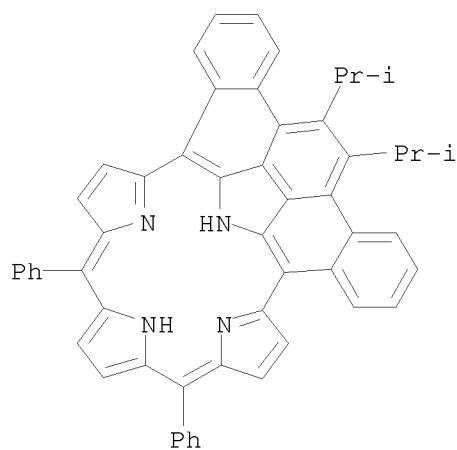
RN 842125-59-1 CAPLUS  
 CN 1,21[1',2']:4,6[1'',2'']-Dibenzeno-23H,25H-benzo[b]porphine,  
 2,3,11,16-tetraphenyl- (9CI) (CA INDEX NAME)



RN 842125-60-4 CAPLUS  
 CN 1,21[1',2']:4,6[1'',2'']-Dibenzeno-23H,25H-benzo[b]porphine,  
 11,16-diphenyl-2,3-dipropyl- (9CI) (CA INDEX NAME)

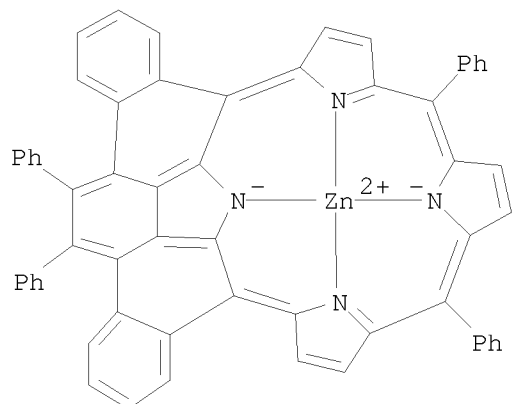


RN	842125-61-5	CAPLUS
CN	1,21[1',2']:4,6[1'',2'']-Dibenzene-23H,25H-benzo[b]porphine, 2,3-bis(1-methylethyl)-11,16-diphenyl- (9CI)	(CA INDEX NAME)

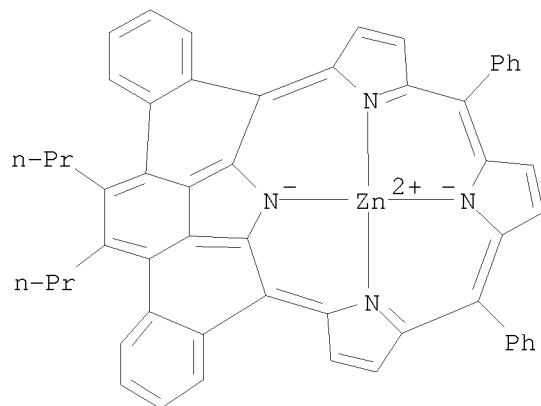


RN	842125-62-6	CAPLUS
CN	Zinc, [2,3,11,16-tetraphenyl-1,21[1',2']:4,6[1'',2'']-dibenzene-23H,25H-benzo[b]porphinato(2-)-κN23,κN24,κN25,κN26]-, (SP-4-1)- (9CI) (CA INDEX NAME)	





RN 842125-63-7 CAPLUS  
 CN Zinc, [11,16-diphenyl-2,3-dipropyl-1,21[1',2']:4,6[1'',2'']-dibenzeno-  
 23H,25H-benzo[b]porphinato(2-)-  
 κN23,κN24,κN25,κN26]-, (SP-4-1)- (9CI) (CA INDEX  
 NAME)



REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 26 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2004:985736 CAPLUS  
 DOCUMENT NUMBER: 142:463488  
 TITLE: The Photodynamic Therapy (PDT) Anticancer Activity of  
 a Range of Porphyrin Dimers and Related Compounds  
 Derived from Hematoporphyrin  
 AUTHOR(S): Byrne, Christopher J.; Cooper, Mathew A.; Cowled,  
 Prudence A.; Johnstone, Robert A. W.; Mackenzie,  
 Lorraine; Marshallsay, Lorely V.; Morris, Ian K.;  
 Muldoon, Craig A.; Raftery, Mark J.; Yin, Sek Sau;  
 Ward, A. David  
 CORPORATE SOURCE: Department of Chemistry, University of Adelaide,  
 Adelaide, SA 5005, Australia  
 SOURCE: Australian Journal of Chemistry (2004), 57(11),

1091-1102

CODEN: AJCHAS; ISSN: 0004-9425

PUBLISHER: CSIRO Publishing

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 142:463488

AB The synthesis of diporphyrins and analogous compds. related to those present in the oligomeric fraction (Photofrin II) obtained from hematoporphyrin derivative (HPD) is described. The photodynamic activity of these compds., in vivo, varies from inactive to as active as Photofrin II. Factors that are important in determining this anticancer activity of the synthetic compds. are the presence of hydrophobic side chains, as well as the propionic acid side chains of the hematoporphyrin derived materials, and the nature of the linking group between the porphyrins.

IT 851440-70-5P

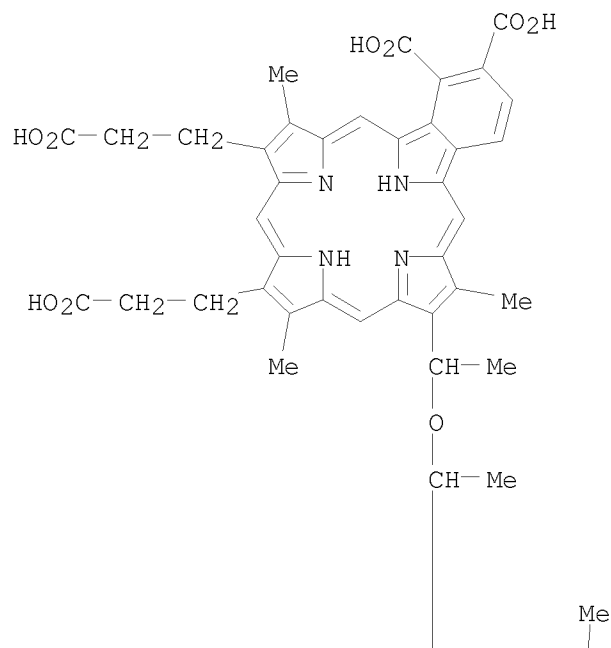
RL: PAC (Pharmacological activity); PNU (Preparation, unclassified); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(photodynamic therapy (PDT) anticancer activity of porphyrin dimers and related compds. derived from hematoporphyrin)

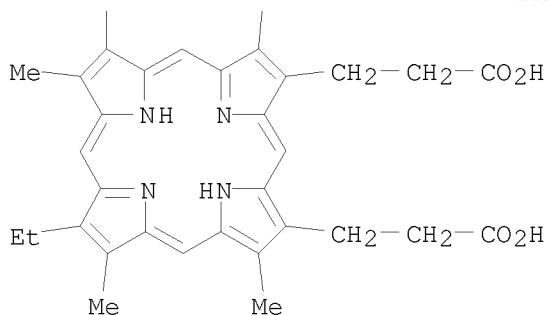
RN 851440-70-5 CAPLUS

CN 23H,25H-Benzo[b]porphine-9,13-dipropionic acid,  
18-[1-[1-[13,17-bis(2-carboxyethyl)-7-ethyl-3,8,12,18-tetramethyl-21H,23H-porphin-2-yl]ethoxy]ethyl]-3,4-dicarboxy-8,14,19-trimethyl- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A

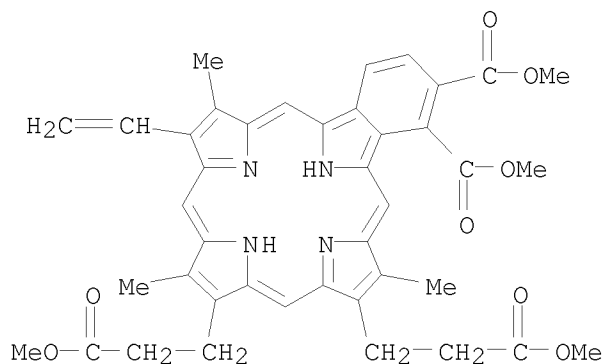


IT 94238-26-3

RL: RCT (Reactant); RACT (Reactant or reagent)

(photodynamic therapy (PDT) anticancer activity of porphyrin dimers and related compds. derived from hematoporphyrin)

RN 94238-26-3 CAPLUS

CN 23H,25H-Benzo[b]porphine-9,13-dipropionic acid,  
18-ethenyl-3,4-bis(methoxycarbonyl)-8,14,19-trimethyl-, dimethyl ester  
(9CI) (CA INDEX NAME)

IT 851441-31-1P

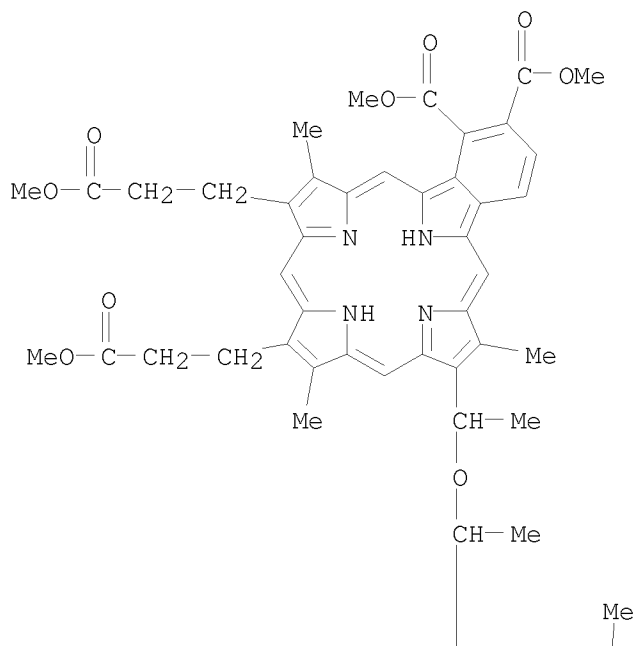
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(photodynamic therapy (PDT) anticancer activity of porphyrin dimers and related compds. derived from hematoporphyrin)

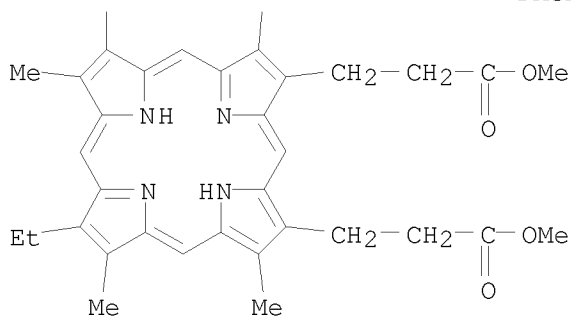
RN 851441-31-1 CAPLUS

CN 23H,25H-Benzo[b]porphine-9,13-dipropionic acid,  
18-[1-[1-[7-ethyl-13,17-bis(3-methoxy-3-oxopropyl)-3,8,12,18-tetramethyl-21H,23H-porphin-2-yl]ethoxy]ethyl]-3,4-bis(methoxycarbonyl)-8,14,19-trimethyl-, dimethyl ester (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



REFERENCE COUNT: 51 THERE ARE 51 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 27 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:498386 CAPLUS

DOCUMENT NUMBER: 141:190619

TITLE: An efficient synthesis of conjugation-expanded carba- and azuliporphyrins using a bicyclo[2.2.2]octadiene-fused tripyrrane

AUTHOR(S): Okujima, Tetsuo; Komobuchi, Naoki; Shimizu, Yusuke; Uno, Hidemitsu; Ono, Noboru

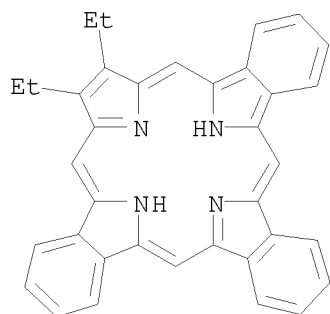
CORPORATE SOURCE: Department of Fundamental Science, Faculty of Science, Ehime University, Matsuyama, 790-8577, Japan

SOURCE: Tetrahedron Letters (2004), 45(28), 5461-5464  
 CODEN: TELEAY; ISSN: 0040-4039  
 PUBLISHER: Elsevier  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 141:190619  
 GI

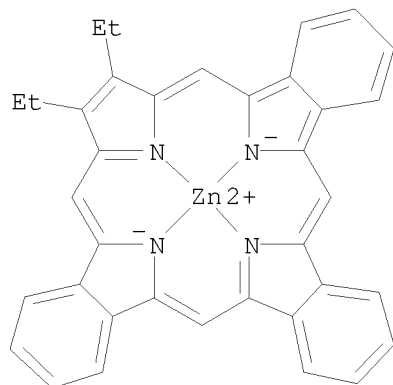
\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB Bicyclo[2.2.2]octadiene-fused tripyrrane I was synthesized as a first versatile reagent for the preparation of  $\pi$ -expanded heteroporphyrins. The reaction of the tripyrrane with 1,3-diformylindene and azulene-1,3-dicarbaldehyde afforded the corresponding heteroporphyrins, e.g. II, which were easily converted into tetrabenzocarbaporphyrin and tribenzoazuliporphyrin by retro Diels-Alder reaction.

IT 736181-67-2P 737766-06-2P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (efficient synthesis of conjugation-expanded carba- and azuliporphyrins using a bicyclo[2.2.2]octadiene-fused tripyrrane)  
 RN 736181-67-2 CAPLUS  
 CN 27H,29H-Tribenzo[b,g,l]porphine, 22,23-diethyl- (9CI) (CA INDEX NAME)



RN 737766-06-2 CAPLUS  
 CN Zinc, [7,8-diethyl-21H,23H-porphinato(2-)-  
 $\kappa$ N21, $\kappa$ N22, $\kappa$ N23, $\kappa$ N24]-, (SP-4-2)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 28 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:354168 CAPLUS

DOCUMENT NUMBER: 141:314039

TITLE: Quasi-line vibronic spectra of 2,3,12,13-tetramethyldibenzoporphine and their interpretation

AUTHOR(S): Solovyov, Konstantin N.; Arabei, Serguei M.; Gladkov, Lev L.; Konstantinova, Vera K.; Turkova, Alisa E.; Avlasevich, Yuri S.

CORPORATE SOURCE: Institute of Molecular and Atomic Physics, National Academy of Sciences of Belarus, Minsk, 220072, Belarus

SOURCE: Journal of Porphyrins and Phthalocyanines (2003), 7(11 & 12), 787-794

CODEN: JPPHFZ; ISSN: 1088-4246

PUBLISHER: Society of Porphyrins & Phthalocyanines

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The quasi-line fluorescence and fluorescence excitation spectra of 2,3,12,13-tetramethyldibenzoporphine have been obtained at 77 K in n-octane and analyzed. The normal-coordinate anal. of this mol. has been performed, and the spectra have been interpreted in detail. In the Soret band region the fluorescence excitation quasi-line spectra clearly reveal two 0-0 components. The problem of the nature of the Soret band of free-base porphyrins is discussed.

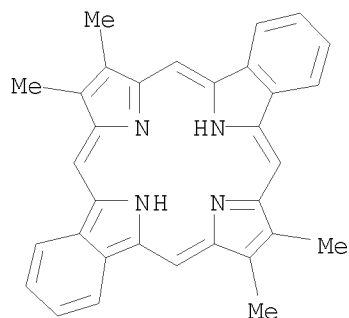
IT 157869-32-4

RL: PRP (Properties)

(quasi-line vibronic spectra of 2,3,12,13-tetramethyldibenzoporphine and their interpretation)

RN 157869-32-4 CAPLUS

CN 25H,27H-Dibenzo[b,l]porphine, 8,9,20,21-tetramethyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 29 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:202762 CAPLUS

DOCUMENT NUMBER: 142:240331

TITLE: Product class 8: porphyrins and related compounds

AUTHOR(S): Smith, K. M.; Vicente, M. G. H.

CORPORATE SOURCE: Louisiana State University, Baton Rouge, LA, 70803-2755, USA

SOURCE: Science of Synthesis (2004), 17, 1081-1235

CODEN: SSCYJ9

PUBLISHER: Georg Thieme Verlag

DOCUMENT TYPE: Journal; General Review

LANGUAGE: English

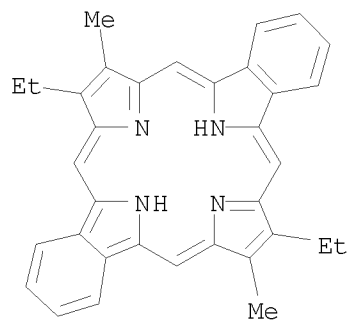
AB A review. Preparation of porphyrins i. e. porphines and related compds. is given.

IT 81976-22-9P 255366-66-6P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of porphyrins and related compds.)

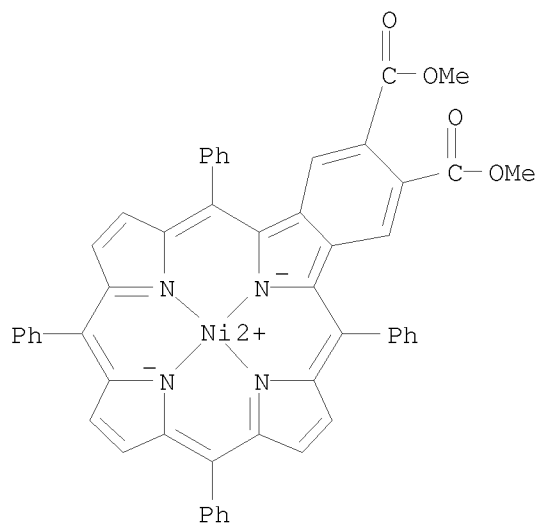
RN 81976-22-9 CAPLUS

CN 25H,27H-Dibenzo[b,l]porphine, 8,20-diethyl-9,21-dimethyl- (9CI) (CA INDEX NAME)



RN 255366-66-6 CAPLUS

CN Nickel, [dimethyl 6,11,16,21-tetraphenyl-23H,25H-benzo[b]porphine-2,3-dicarboxylato(2-)-κN23,κN24,κN25,κN26]-, (SP-4-1)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 577 THERE ARE 577 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

L9 ANSWER 30 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2003:971163 CAPLUS  
 DOCUMENT NUMBER: 140:21921  
 TITLE: Organic semiconductor material and organic electronic device  
 INVENTOR(S): Aramaki, Shinji; Ono, Noboru  
 PATENT ASSIGNEE(S): Mitsubishi Chemical Corporation, Japan  
 SOURCE: U.S. Pat. Appl. Publ., 39 pp.  
 CODEN: USXXCO  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 2  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20030226996	A1	20031211	US 2003-396512	20030326
US 7193237	B2	20070320		
JP 2003304014	A	20031024	JP 2002-104639	20020408
JP 2004006750	A	20040108	JP 2003-84816	20030326
US 20070145361	A1	20070628	US 2007-671085	20070205
JP 2008270843	A	20081106	JP 2008-205635	20080808
PRIORITY APPLN. INFO.:			JP 2002-89425	A 20020327
			JP 2002-104639	A 20020408
			JP 2003-84816	A3 20030326
			US 2003-396512	A3 20030326

AB An organic semiconductor material which has high carrier mobility and stability and which can be formed into a film by a simple production process such as a coating process, and an organic electronic device employing such an organic semiconductor material is claimed. An organic semiconductor material comprising a compound which has a generalized porphyrin skeleton and which has a mol. structure such that the distance from the generalized porphyrin



ring plane to the center of each atom forming the generalized porphyrin skeleton, is  $\leq 1$  Å.

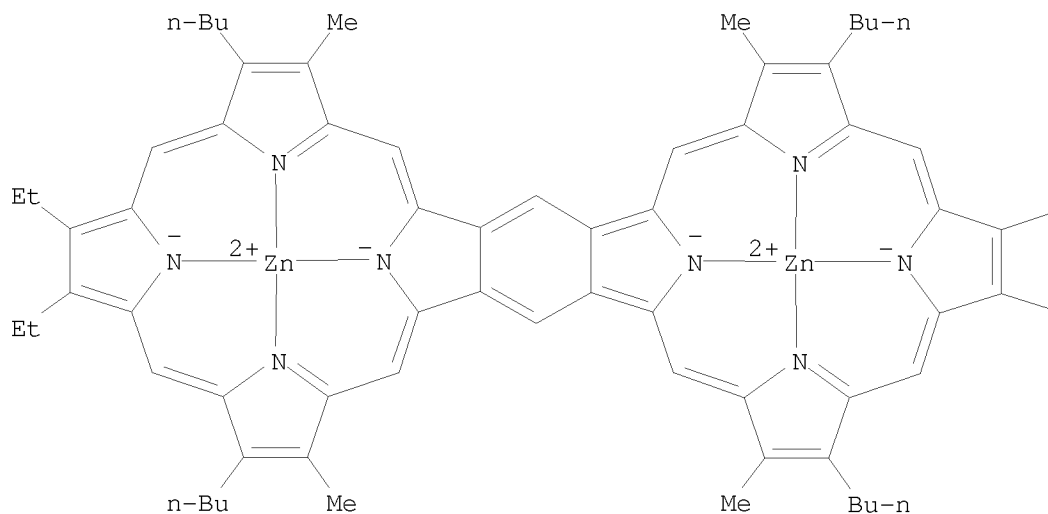
IT 406483-35-0P

RL: DEV (Device component use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)  
(preparation and devices from)

RN 406483-35-0 CAPLUS

CN Zinc, [ $\mu$ -[5,14,24,33-tetrabutyl-9,10,28,29-tetraethyl-4,15,23,34-tetramethyl-39H,41H,43H,45H-benzo[1,2-b:4,5-b']diporphinato(4-)- $\kappa$ N39, $\kappa$ N40, $\kappa$ N41, $\kappa$ N42: $\kappa$ N43, $\kappa$ N44, $\kappa$ N45, $\kappa$ N46]]di- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B

Et

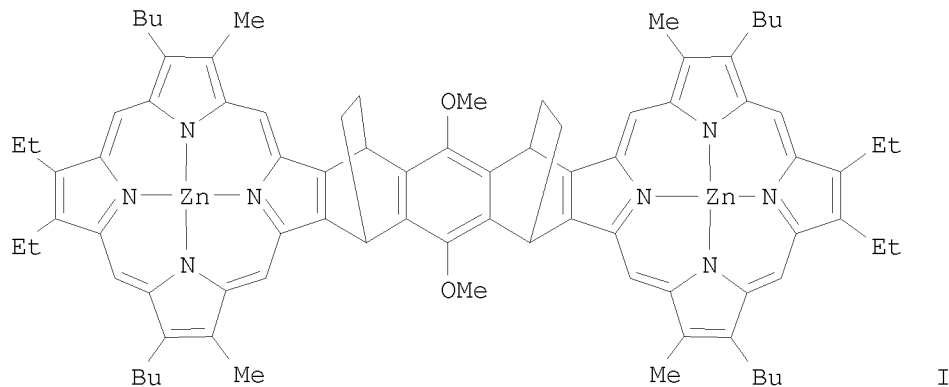
Et

REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 31 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2003:724055 CAPLUS

DOCUMENT NUMBER: 139:316045  
 TITLE: Hexagonal Columnar Porphyrin Assembly by Unique Trimeric Complexation of a Porphyrin Dimer with  $\pi$ - $\pi$  Stacking: Remarkable Thermal Behavior in a Solid  
 AUTHOR(S): Uno, Hidemitsu; Masumoto, Akane; Ono, Noboru  
 CORPORATE SOURCE: Division of Synthesis and Analysis, Department of Molecular Science, Integrated Center for Sciences (INCS), Ehime University, Matsuyama, 790-8577, Japan  
 SOURCE: Journal of the American Chemical Society (2003), 125(40), 12082-12083  
 CODEN: JACSAT; ISSN: 0002-7863  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 139:316045  
 GI



AB Syn- and anti-I were prepared and characterized by single crystal structural anal. On heating, syn-I, the crystal structure of which showed a unique trimeric assembly, lost an ethylene mol. at 240-310° to give a porphyrin-naphthoporphyrin diad, and the 2nd Diels-Alder reaction and concomitant decomposition of the methoxy groups occurred at 280-350° to the anthraquinone derived diporphyrin, while the 1st thermal conversion of anti-I occurred in a much low temperature range (180-230°). Syn- exhibits hexagonal columnar --stacking interaction which may explain the difference in thermal behavior.

IT 610269-60-8P 610269-61-9P

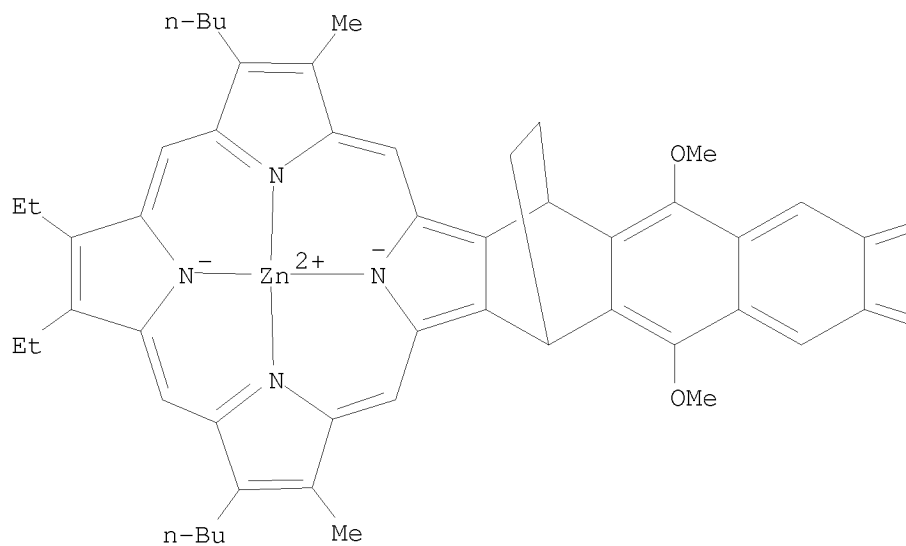
RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation from thermal decomposition of zinc complexes with porphyrin having fused di(ethano)anthracene)

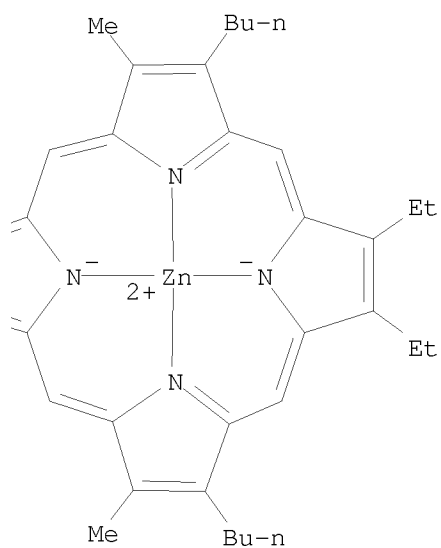
RN 610269-60-8 CAPLUS

CN Zinc, [ $\mu$ -[5,14,26,35-tetrabutyl-9,10,30,31-tetraethyl-19,42-dihydro-20,41-dimethoxy-4,15,25,36-tetramethyl-19,42-ethano-43H,45H,47H,49H-anthra[2,3-b:6,7-b']diporphinato(4-)- $\kappa$ N43, $\kappa$ N44, $\kappa$ N45, $\kappa$ N46: $\kappa$ N47, $\kappa$ N48, $\kappa$ N49, $\kappa$ N50]]di- (9CI) (CA INDEX NAME)

PAGE 1-A

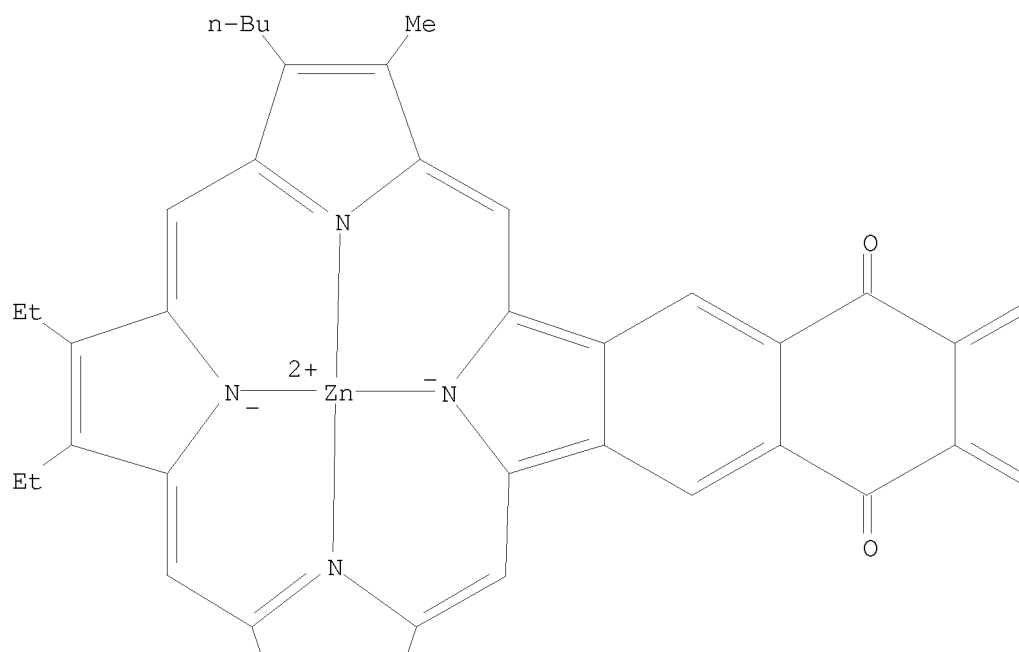


PAGE 1-B

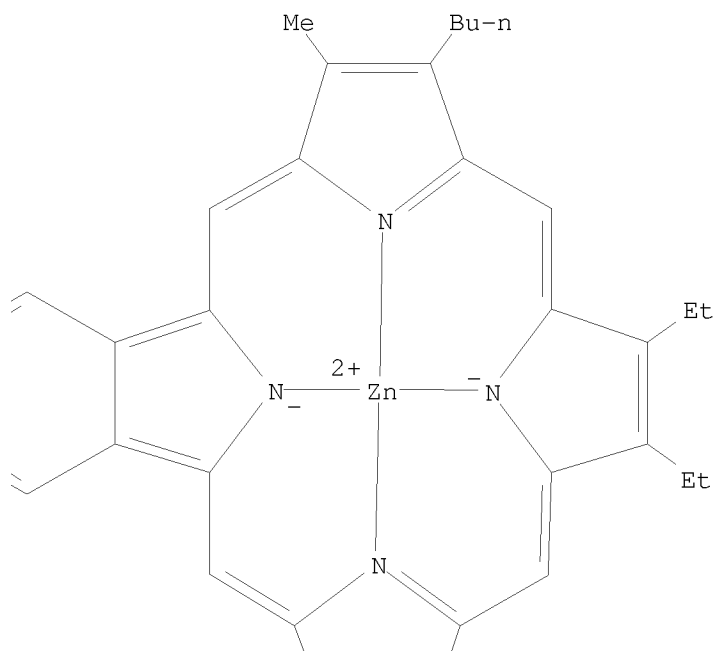


RN 610269-61-9 CAPLUS  
 CN Zinc, [ $\mu$ -[5,14,26,35-tetrabutyl-9,10,30,31-tetraethyl-4,15,25,36-tetramethyl-43H,45H,47H,49H-anthra[2,3-b:6,7-b']diporphine-20,41-dionato(4-)- $\kappa$ N43, $\kappa$ N44, $\kappa$ N45, $\kappa$ N46: $\kappa$ N47, $\kappa$ N48,.kappa.N49, $\kappa$ N50]]di- (9CI) (CA INDEX NAME)

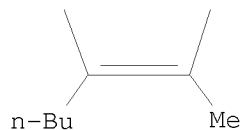
PAGE 1-A



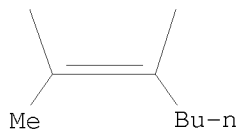
PAGE 1-B



PAGE 2-A

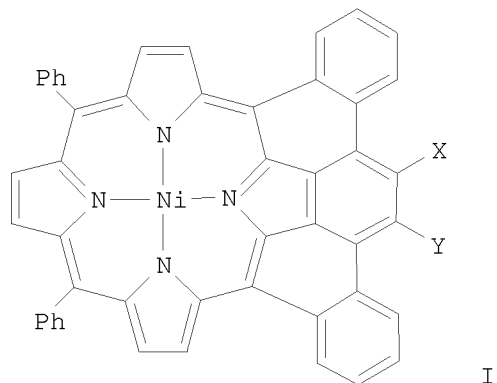


PAGE 2-B

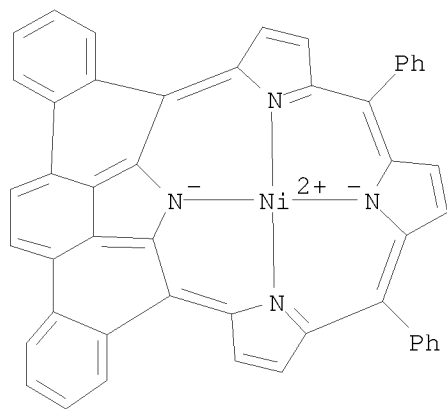


REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 32 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2003:681122 CAPLUS  
 DOCUMENT NUMBER: 139:285109  
 TITLE: Ambient Temperature Activation of Haloporphyrinic-Enediynes: Electronic Contributions to Bergman Cycloaromatization  
 AUTHOR(S): Nath, Mahendra; Huffman, John C.; Zaleski, Jeffrey M.  
 CORPORATE SOURCE: Department of Chemistry, Indiana University, Bloomington, IN, 47405, USA  
 SOURCE: Journal of the American Chemical Society (2003), 125(38), 11484-11485  
 CODEN: JACSAT; ISSN: 0002-7863  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 139:285109  
 GI

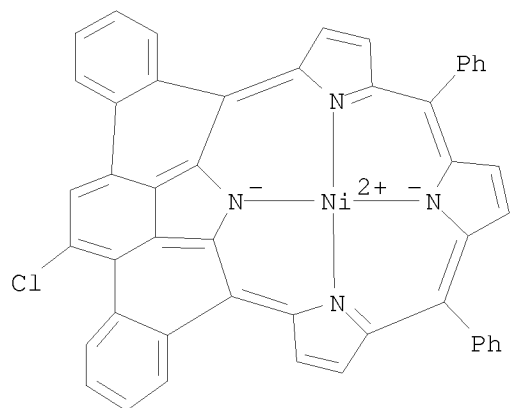


- AB The authors synthesized the nickel(II) 2,3-bis(haloethynyl)-5,10,15,20-tetraphenylporphyrins with -Br (2a) or -I (2b) at the alkyne termini position from the corresponding 2,3-diethynyl analog (1). The cross coupling of nickel(II) 2,3-dibromo-5,10,15,20-tetraphenylporphyrin with trimethyl(trimethylstannanylethynyl)silane in the presence of a Pd0 catalyst and subsequent deprotection with base under aqueous conditions yields the nickel(II) 2,3-diethynyl-5,10,15,20-tetraphenylporphyrin (1). Subsequent reaction of 1 with N-bromo- or N-iodosuccinimide in dry acetone in the presence of AgNO<sub>3</sub> yields 2,3-bis(haloethynyl)-5,10,15,20-tetraphenylporphyrins in 70% (2a) and 68% (2b) yields. The x-ray crystal structures of 2a,b show that the porphyrin backbone deviates significantly from planarity due to a Ni(II)-induced mixture of the classic ruffle and saddle distortions. Thermolysis of 2a at 190° for 6 h in chlorobenzene and 30-fold 1,4-cyclohexadiene (CHD) generates the Bergman cyclized nickel(II) dibromopicenoporphyrin product (3: I, X = Y = Br) in 65% yield, which derives from diradical addition across the adjacent meso-Ph substituents. Similarly, nickel(II) 2,3-bis(iodoethynyl)-5,10,15,20-tetraphenylporphyrin, 2b, cyclizes at 190° in chlorobenzene/CHD via high-temperature substitution of iodine by hydrogen (from CHD) or chlorine (from solvent) to afford a mixture of 4 (I, X = Y = H, 15%) and 5 (I, X = H, Y = Cl, 45%). Remarkably, ambient temperature incubation of 2a in MeOH/CHCl<sub>3</sub> (1:3, 22 h) or chlorobenzene/CHD (3:1, 24 h) gives 3 in 15% and 22% isolated yields, resp. Addition of 1.2 equiv of 2,3-dichloro-5,6-dicyano-1,4-benzoquinone (DDQ) in CHCl<sub>3</sub>/MeOH dramatically accelerates the rate of reaction, producing 3 in 30% yield within 0.5 h. The origin of the ambient temperature activation of 2a derives from the ability of electron-withdrawing functionalities at the alkyne termini to decrease the activation barrier to the Bergman product.
- IT 380447-58-5P 607391-89-9P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation by Bergman cycloaromatization)
- RN 380447-58-5 CAPLUS
- CN Nickel, [11,16-diphenyl-1,21[1',2']:4,6[1'',2'']-dibenzeno-23H,25H-benzo[b]porphinato(2-)-κN23,κN24,κN25,κN26]-, (SP-4-1)- (9CI) (CA INDEX NAME)

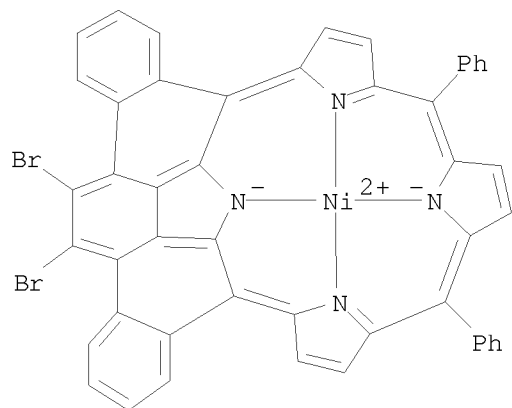


RN 607391-89-9 CAPLUS

CN Nickel, [2-chloro-11,16-diphenyl-1,21[1',2']:4,6[1'',2'']-dibenzeno-23H,25H-benzo[b]porphinato(2-)-κN23,κN24,κN25,κN26]-, (SP-4-2)- (9CI) (CA INDEX NAME)



IT 607391-88-8P 607391-95-7P  
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
 (preparation by Bergman cycloaromatization and crystal and mol. structure)  
 RN 607391-88-8 CAPLUS  
 CN Nickel, [2,3-dibromo-11,16-diphenyl-1,21[1',2']:4,6[1'',2'']-dibenzeno-23H,25H-benzo[b]porphinato(2-)-κN23,κN24,κN25,κN26]-, (SP-4-1)- (9CI) (CA INDEX NAME)

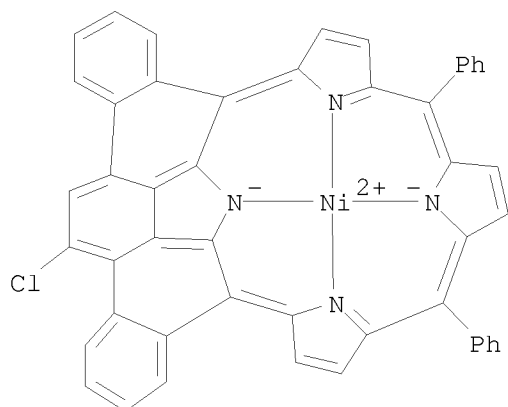


RN 607391-95-7 CAPLUS  
 CN Nickel, [2-chloro-11,16-diphenyl-1,21[1',2']:4,6[1'',2'']-dibenzeno-23H,25H-benzo[b]porphinato(2-)-κN23,κN24,κN25,κN26]-, (SP-4-2)-, compd. with benzene (4:3) (9CI) (CA INDEX NAME)

CM 1

CRN 607391-89-9

CMF C48 H25 Cl N4 Ni  
CCI CCS



CM 2

CRN 71-43-2  
CMF C6 H6



REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 33 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2003:238771 CAPLUS

DOCUMENT NUMBER: 139:117243

TITLE: Accelerated Bergman cyclization of porphyrinic-enediynes

AUTHOR(S): Nath, Mahendra; Huffman, John C.; Zaleski, Jeffrey M.

CORPORATE SOURCE: Department of Chemistry, Indiana University, Bloomington, IN, USA

SOURCE: Chemical Communications (Cambridge, United Kingdom) (2003), (7), 858-859

CODEN: CHCOFS; ISSN: 1359-7345

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 139:117243

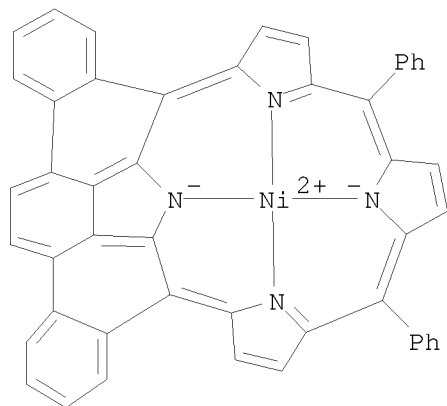
AB The Bergman cyclization of simple diethynylporphyrinic-enediynes exhibits a double activation barrier to the formation of Bergman cyclized products. Addition of H-atom acceptor accelerates the formation of the picenoporphyrin, indicating that the second barrier is rate limiting.

IT 380447-58-5P 564475-27-0P

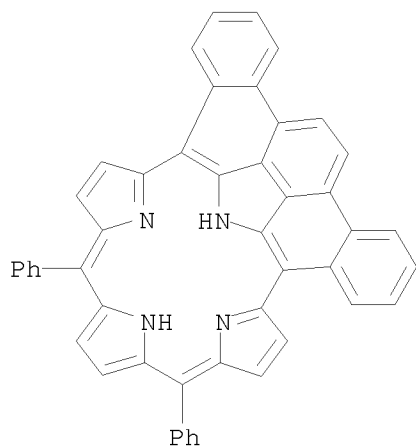
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (crystal structure; accelerated Bergman cyclization of



porphyrinic-enediynes)  
 RN 380447-58-5 CAPLUS  
 CN Nickel, [11,16-diphenyl-1,21[1',2']:4,6[1'',2'']-dibenzeno-23H,25H-  
 benzo[b]porphinato(2-)-κN23,κN24,κN25,κN26]-,  
 (SP-4-1)- (9CI) (CA INDEX NAME)



RN 564475-27-0 CAPLUS  
 CN 1,21[1',2']:4,6[1'',2'']-Dibenzeno-23H,25H-benzo[b]porphine,  
 11,16-diphenyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

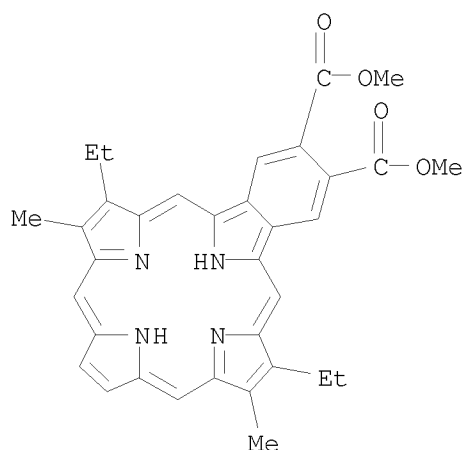
L9 ANSWER 34 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2003:151529 CAPLUS  
 DOCUMENT NUMBER: 139:6702  
 TITLE: Establishing a library of porphyrin building blocks  
 for superstructured assemblies: Porphyrin dienes and  
 dienophiles for cycloaddition reactions  
 AUTHOR(S): Gunter, Maxwell J.; Tang, Hesheng; Warrenner, Ronald N.  
 CORPORATE SOURCE: Division of Chemistry, University of New England,

SOURCE: Armidale, NSW 2351, Australia  
 Journal of Porphyrins and Phthalocyanines (2002), 6(11 & 12), 673-684  
 CODEN: JPPHFZ; ISSN: 1088-4246  
 PUBLISHER: Society of Porphyrins & Phthalocyanines  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 139:6702

AB The synthesis and utility of a series of porphyrins with (masked) diene and dienophile functionality are described. The key porphyrin diene is synthesized from a sulfolenopyrrole by a 3+1 strategy. A range of Diels-Alder cycloadducts is readily accessed from the diene by mild thermal extrusion of sulfur dioxide from the sulfolenoporphyrin, which produces the reactive porphodimethylidene. Each of these cycloadducts is fused to the porphyrin nucleus through a cyclohexene ring thus retaining some conformational flexibility in the resultant structures. The structures can be rigidified by mild oxidation to the corresponding benzo-derivs. Diels-Alder reaction of the porphyrin 1,3-diene resulting from the sulfolenoporphyrin with norbornadiene produces the norbornene derivative, which can serve as a dienophile or dipolarophile in subsequent cycloaddn. reactions. Nevertheless, a preferred route to this structure is through a corresponding 1+3 route, where the norbornene component is part of the tripyrrane. Extension of the synthetic protocols allows ready access to a "mixed function" porphyrin, containing both diene and dienophile components. Likewise, the synthesis of a bis-norbornene porphyrin is described. A collection of each of these reactive components is the basis for a library of building blocks which allows easy and simple entry to a wide variety of complex porphyrin-containing superstructures.

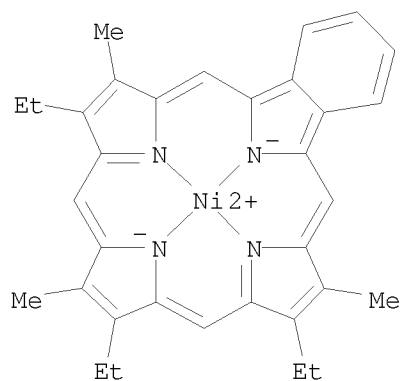
IT 532993-93-4P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (establishing a library of porphyrin dienes and dienophiles for cycloaddn. reactions)

RN 532993-93-4 CAPLUS  
 CN 23H,25H-Benzo[b]porphine-2,3-dicarboxylic acid,  
 8,19-diethyl-9,18-dimethyl-, dimethyl ester (9CI) (CA INDEX NAME)



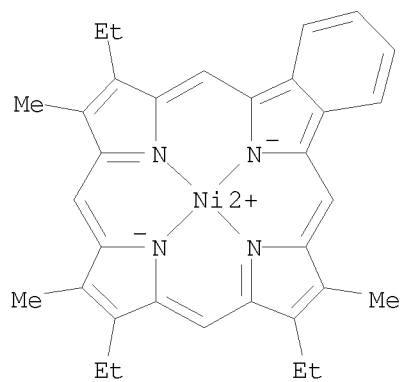
REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 35 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 2002:631085 CAPLUS  
DOCUMENT NUMBER: 138:92379  
TITLE: Fingerprinting petroporphyrin structures with  
vibrational spectroscopy. Part 6: resonance Raman  
characterization of regioisomers of nickel(II)  
benzoetioporphyrin  
AUTHOR(S): Boggess, James M.; Czernuszewicz, Roman S.; Lash,  
Timothy D.  
CORPORATE SOURCE: Department of Chemistry, University of Houston,  
Houston, TX, 77204-5003, USA  
SOURCE: Organic Geochemistry (2002), 33(9), 1111-1126  
CODEN: ORGEDE; ISSN: 0146-6380  
PUBLISHER: Elsevier Science Ltd.  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB Nickel(II) complexes of the geochem. significant four regioisomers of  
benzoetioporphyrin, Ni(BP-A-D), which contain a benzene ring fused onto  
the C $\beta$  atoms of a pyrrole ring, have been synthesized and  
structurally characterized by resonance Raman spectroscopy. Laser  
excitations in resonance with the porphyrin Soret (406.7 nm) and Q (530.9  
and 568.2 nm) electronic absorption bands exposed nearly all Raman active  
vibrations in the fingerprint region (100-1700 cm<sup>-1</sup>). The porphyrin  
skeletal vibrations above 1300 cm<sup>-1</sup> are largely unaffected by the  
different location of the  $\beta,\beta$ -benzo exocyclic ring, but their  
frequencies indicate slightly more planar structures in solution for Ni(BP)  
porphyrins relative to nickel tetrahydrobenzo- and etioporphyrins.  
Several unique marker bands are also found for vibrations of the  
 $\beta,\beta$ -benzo substituent, especially in the Soret-band resonant spectra.  
Alkyl substituent and porphyrin skeletal vibrations in the low- (350-550  
cm<sup>-1</sup>) and mid-frequency (750-1300 cm<sup>-1</sup>) regions show striking sensitivity  
to small conformational changes in the porphyrin, allowing the four Ni(BP)  
regioisomers to be readily distinguished.  
IT 483979-43-7 483979-44-8 483979-45-9  
483979-46-0  
RL: ANT (Analyte); PRP (Properties); ANST (Analytical study)  
(resonance Raman spectra of regioisomers of nickel(II)  
benzoetioporphyrin)  
RN 483979-43-7 CAPLUS  
CN Nickel, [9,14,18-triethyl-8,13,19-trimethyl-23H,25H-benzo[b]porphinato(2-)-  
 $\kappa$ N23, $\kappa$ N24, $\kappa$ N25, $\kappa$ N26]-, (SP-4-2)- (9CI) (CA INDEX  
NAME)



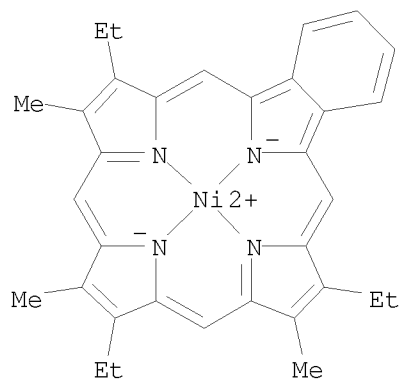
RN 483979-44-8 CAPLUS

CN Nickel, [8,14,18-triethyl-9,13,19-trimethyl-23H,25H-benzo[b]porphinato(2-)-  
κN23,κN24,κN25,κN26]-, (SP-4-2)- (9CI) (CA INDEX  
NAME)

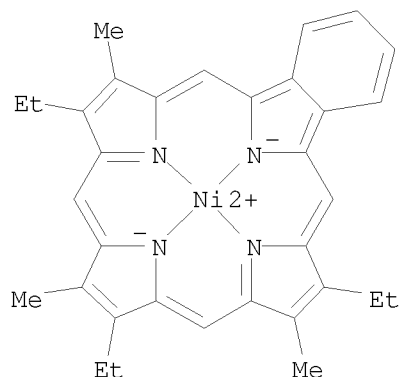


RN 483979-45-9 CAPLUS

CN Nickel, [8,13,19-triethyl-9,14,18-trimethyl-23H,25H-benzo[b]porphinato(2-)-  
κN23,κN24,κN25,κN26]-, (SP-4-2)- (9CI) (CA INDEX  
NAME)

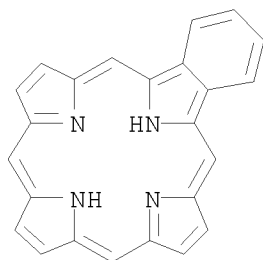


RN 483979-46-0 CAPLUS  
 CN Nickel, [8,13,18-triethyl-9,14,19-trimethyl-23H,25H-benzo[b]porphinato(2-)-  
 κN23,κN24,κN25,κN26]-, (SP-4-2)- (9CI) (CA INDEX  
 NAME)

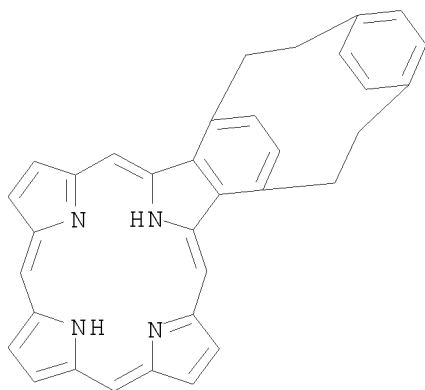


REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 36 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2002:525234 CAPLUS  
 DOCUMENT NUMBER: 137:369676  
 TITLE: Theoretical optical spectra of some  
 [22](1,4)-cyclophane fused tetraazaporphyrins  
 AUTHOR(S): Turker, Lemi  
 CORPORATE SOURCE: Department of Chemistry, Middle East Technical  
 University, Ankara, 06531, Turk.  
 SOURCE: THEOCHEM (2002), 588, 133-138  
 CODEN: THEODJ; ISSN: 0166-1280  
 PUBLISHER: Elsevier Science B.V.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB ZINDO/S type semiempirical MO calcns. were carried out on the benzo and  
 [22](1,4)-cyclophane fused tetraazaporphyrins. The phane deck is  
 influential on UV-visible singlet transitions causing some bathochromic  
 shifts.  
 IT 36469-17-7, 23H,25H-Benzo[b]porphine 475595-26-7  
 RL: PRP (Properties)  
 (theor. optical spectra of some [22](1,4)-cyclophane fused  
 tetraazaporphyrins)  
 RN 36469-17-7 CAPLUS  
 CN 23H,25H-Benzo[b]porphine (9CI) (CA INDEX NAME)

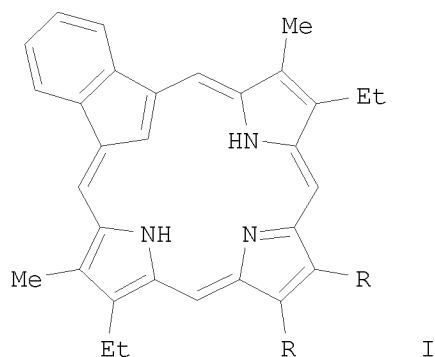


RN 475595-26-7 CAPLUS  
 CN 1,10:4,7-Dietheno-29H,31H-cyclododeca[b]porphine, 2,3,8,9-tetrahydro-  
 (9CI) (CA INDEX NAME)



REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 37 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2002:406065 CAPLUS  
 DOCUMENT NUMBER: 137:140367  
 TITLE: Conjugated Macrocycles Related to the Porphyrins.  
 21.Synthesis, Spectroscopy, Electrochemistry, and  
 Structural Characterization of Carbaporphyrins  
 AUTHOR(S): Lash, Timothy D.; Hayes, Michael J.; Spence, John D.;  
 Muckey, Melanie A.; Ferrence, Gregory M.; Szczepura,  
 Lisa F.  
 CORPORATE SOURCE: Department of Chemistry, Illinois State University,  
 Normal, IL, 61790-4160, USA  
 SOURCE: Journal of Organic Chemistry (2002), 67(14), 4860-4874  
 CODEN: JOCEAH; ISSN: 0022-3263  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 137:140367  
 GI



AB The "3 + 1" variant of the MacDonald condensation has been shown to be an excellent methodol. for synthesizing carbaporphyrins. In particular, 1,3-indenedicarbaldehyde condenses with tripyrranes in the presence of TFA to give, following oxidation with DDQ, a series of benzocarbaporphyrins in excellent yields. Triformylcyclopentadienes also afford carbaporphyrin products, albeit in low yields ranging from 5 to 8%. These hybrid bridged annulene structures have porphyrin-like electronic absorption spectra with strong Soret bands near 420 nm and a series of Q-bands through the visible region. The proton NMR spectrum confirms the presence of a strong diamagnetic ring current, and the meso-protons show up at 10 ppm, while the internal CH is shielded to approx. -7 ppm. Carbaporphyrins undergo reversible protonation with TFA. Initial addition of acid affords a monocation, although mixts. of protonated species are observed in the presence of moderate concns. of TFA. However, in the presence of 50% TFA a C-protonated dication is generated. The dications relocate the  $\pi$ -delocalization pathway through the benzo moiety of benzocarbaporphyrins, and these therefore represent bridged benzo[18]annulenes, although they nevertheless retain powerful macrocyclic ring currents. Carbaporphyrins with fused acenaphthylene and phenanthrene rings have been prepared, and the former demonstrated significantly larger bathochromic shifts in UV-vis spectroscopy that parallel previous observations for acenaphthoporphyrins. A diphenyl-substituted benzocarbaporphyrin I (R = Ph) was also characterized by X-ray crystallog., and these data show that the macrocycle is reasonably planar although the indene subunit is tilted out of the mean macrocyclic plane by 15.5°. The structural data indicates that the preferred tautomer in the solid state has the two NH's flanking the pyrrole unit in agreement with previous spectroscopic and theor. studies. Cyclic voltammetry for carbaporphyrin I (R = Et) was more complex than for true porphyrins, showing five anodic waves and two quasi-reversible reductive couples.

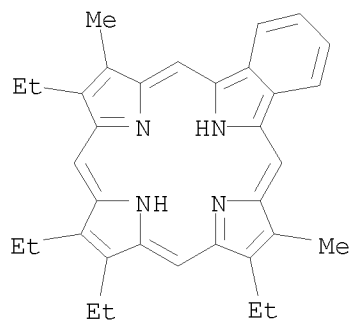
IT 444586-48-5 444586-70-3

RL: PRP (Properties)

(preparation of carbaporphyrins via MacDonald condensation, their UV-visible spectra, cyclic voltammetry, and structure)

RN 444586-48-5 CAPLUS

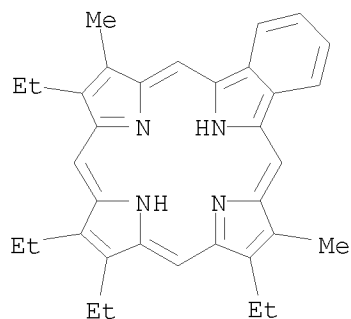
CN 23H,25H-Benzo[b]porphine, 9,13,14,18-tetraethyl-8,19-dimethyl- (9CI) (CA INDEX NAME)



RN 444586-70-3 CAPLUS  
 CN 23H,25H-Benzo[b]porphine, 9,13,14,18-tetraethyl-8,19-dimethyl-,  
 mono(trifluoroacetate) (9CI) (CA INDEX NAME)

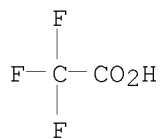
CM 1

CRN 444586-48-5  
 CMF C34 H36 N4



CM 2

CRN 76-05-1  
 CMF C2 H F3 O2

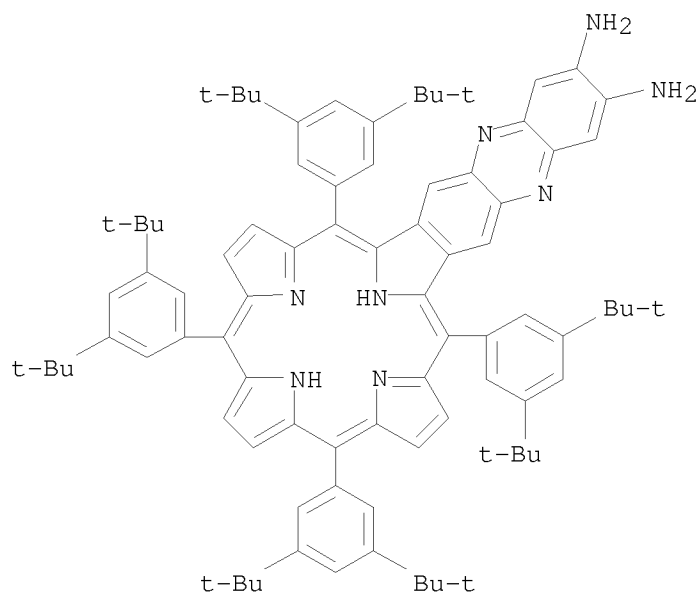


REFERENCE COUNT: 121 THERE ARE 121 CITED REFERENCES AVAILABLE FOR  
 THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE  
 FORMAT

L9 ANSWER 38 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2002:356333 CAPLUS  
 DOCUMENT NUMBER: 137:208912



TITLE: Laterally-extended porphyrin systems incorporating a switchable unit  
 AUTHOR(S): Crossley, Maxwell J.; Johnston, Lesley A.  
 CORPORATE SOURCE: School of Chemistry, The University of Sydney, 2006, Australia  
 SOURCE: Chemical Communications (Cambridge, United Kingdom) (2002), (10), 1122-1123  
 CODEN: CHCOFS; ISSN: 1359-7345  
 PUBLISHER: Royal Society of Chemistry  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB P-Quinone units incorporated into the central portion of rigid  $\pi$ -systems linking either two porphyrin macrocycles or a porphyrin and a phenanthroline group have the potential to function as a chemical and electrochem. controllable switch, thus acting as a means of modulating electronic communication between the two end groups.  
 IT 245445-24-3  
 RL: PRP (Properties)  
 (electronic spectrum of)  
 RN 245445-24-3 CAPLUS  
 CN 27H,29H-Phenazino[2,3-b]porphine-2,3-diamine, 8,13,18,21-tetrakis[3,5-bis(1,1-dimethylethyl)phenyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 39 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2001:928125 CAPLUS  
 DOCUMENT NUMBER: 136:288101  
 TITLE: Synthesis of a gable bis-porphyrin linked with a bicyclo[2.2.2]octadiene ring and its conversion into a conjugated planar bis-porphyrin

AUTHOR(S): Ito, Satoshi; Nakamoto, Ken-ichi; Uno, Hidemitsu;  
 Murashima, Takashi; Ono, Noboru  
 CORPORATE SOURCE: Department of Chemistry, Faculty of Science, Ehime  
 University, Matsuyama, 790-8577, Japan  
 SOURCE: Chemical Communications (Cambridge, United Kingdom)  
 (2001), (24), 2696-2697  
 CODEN: CHCOFS; ISSN: 1359-7345  
 PUBLISHER: Royal Society of Chemistry  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 136:288101  
 GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB The dinuclear zinc complex of a soluble porphyrin dimer linked with  
 bicyclo[2.2.2]octadiene (I) was converted into insol. conjugated porphyrin  
 dimer (II) by heating at 200°; this provides a new strategy for the  
 process control of conjugated porphyrins.

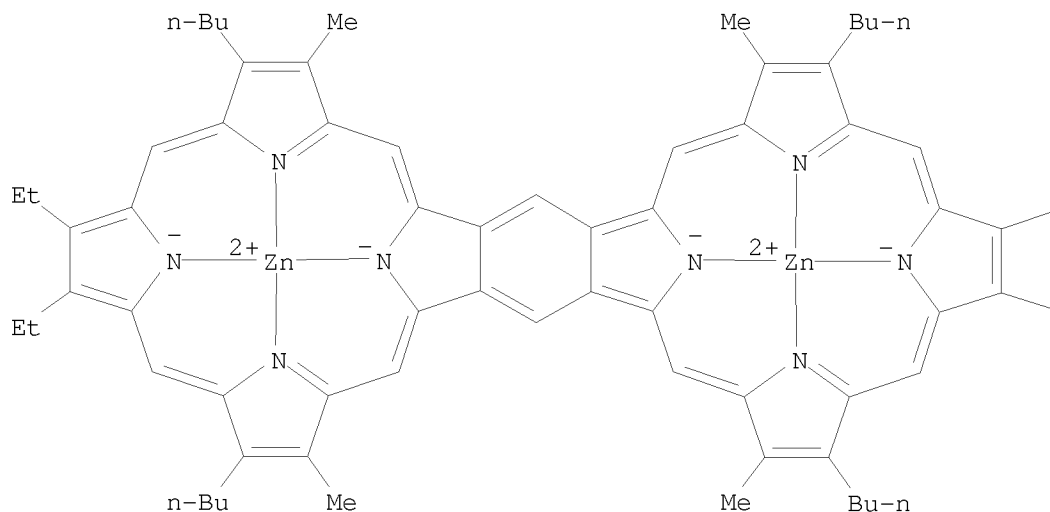
IT 406483-35-0P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)

RN 406483-35-0 CAPLUS

CN Zinc, [ $\mu$ -[5,14,24,33-tetrabutyl-9,10,28,29-tetraethyl-4,15,23,34-  
 tetramethyl-39H,41H,43H,45H-benzo[1,2-b:4,5-b']diporphinato(4-)-  
 $\kappa$ N39, $\kappa$ N40, $\kappa$ N41, $\kappa$ N42: $\kappa$ N43, $\kappa$ N44, $\kappa$ N  
 45, $\kappa$ N46]]di- (9CI) (CA INDEX NAME)

PAGE 1-A



Et

Et

REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 40 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2001:755288 CAPLUS

DOCUMENT NUMBER: 136:207539

TITLE: Singlet oxygen formation and photostability of meso-tetraarylporphyrin derivatives and their copper complexes

AUTHOR(S): Cavaleiro, Jose A. S.; Gorner, Helmut; Lacerda, Paula S. S.; MacDonald, J. Gavin; Mark, Gertraud; Neves, Maria G. P. M. S.; Nohr, Ronald S.; Schuchmann, Heinz-Peter; von Sonntag, Clemens; Tome, Augusto C.

CORPORATE SOURCE: Department of Chemistry, University of Aveiro, Aveiro, 3810-193, Port.

SOURCE: Journal of Photochemistry and Photobiology, A: Chemistry (2001), 144(2-3), 131-140  
CODEN: JPPCEJ; ISSN: 1010-6030

PUBLISHER: Elsevier Science S.A.

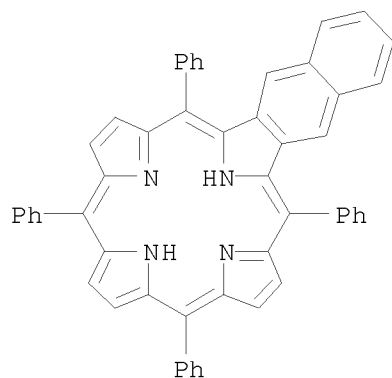
DOCUMENT TYPE: Journal

LANGUAGE: English

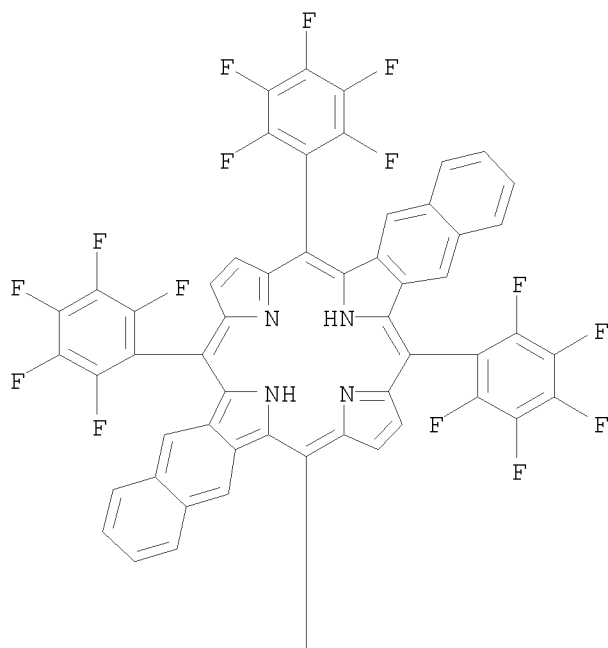
AB Time-resolved photochem. studies of five porphyrin derivs. and their copper complexes were carried out. Triplet lifetimes (room temperature) were determined under argon, air, and oxygen. The presence of oxygen and copper shortens the triplet lifetimes (Ar: in the order of 102  $\mu$ s) by up to three orders of magnitude. With the copper complexes,  $\Phi[O_2(1\Delta_g)]$  is lower than with the metal-free porphyrins. The photodegrdn., indicated by bleaching, of meso-tetraphenylporphyrin and meso-tetrakis(pentafluorophenyl)porphyrin under air shows the latter to be more stable than the former, and their copper complexes to be more stable than the porphyrins themselves. With meso-tetraphenylporphyrin, the effect depends on the solvent, especially in the absence of oxygen (bleaching

is faster in toluene than in benzene). With meso-tetraphenylporphyrin in toluene ( $\lambda_{irr} = 405$  nm), the quantum yields of bleaching, determined from the rate of fading of the maximum of the Soret band are vs. .apprx.  $1.8 \times 10^{-4}$  (Ar) and .apprx.  $1.1 \times 10^{-5}$  ( $O_2$ ). Two rate consts. have been roughly estimated: (i) for the H-atom abstraction from toluene by the triplet excited meso-tetraphenylporphyrin, in the order of  $0.1 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ ; (ii) for the product-forming reaction of  $O_2(1\Delta_g)$  with meso-tetraphenylporphyrin,  $40 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ .

IT 193283-52-2 401510-86-9 401512-05-8  
 401512-06-9  
 RL: CPS (Chemical process); PEP (Physical, engineering or chemical  
 process); PRP (Properties); PROC (Process)  
 (singlet oxygen formation and photostability of meso-tetraarylporphyrin  
 derivs. and their copper complexes)  
 RN 193283-52-2 CAPLUS  
 CN 25H,27H-Naphtho[2,3-b]porphine, 7,12,17,22-tetraphenyl- (CA INDEX NAME)

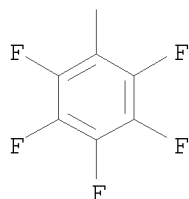


RN 401510-86-9 CAPLUS  
 CN 29H,31H-Dinaphtho[2,3-b:2',3'-1]porphine,  
 7,12,21,26-tetrakis(pentafluorophenyl)- (9CI) (CA INDEX NAME)

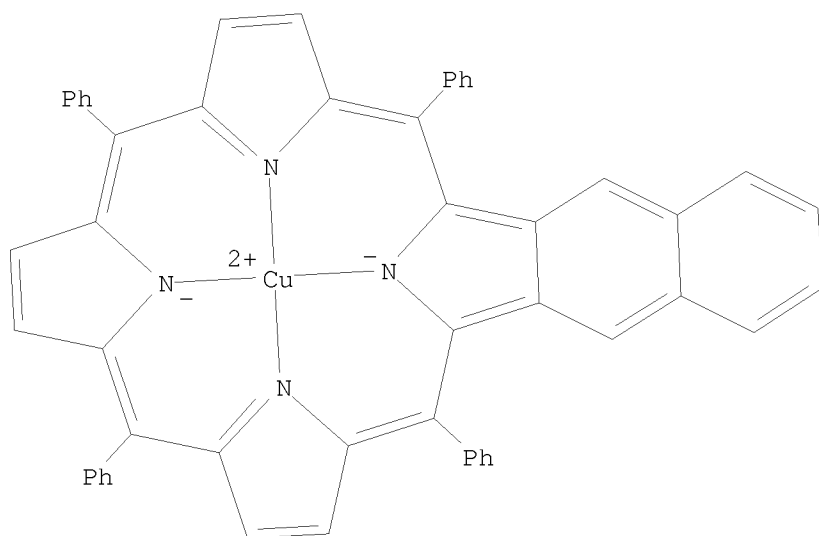


PAGE 1-A

PAGE 2-A

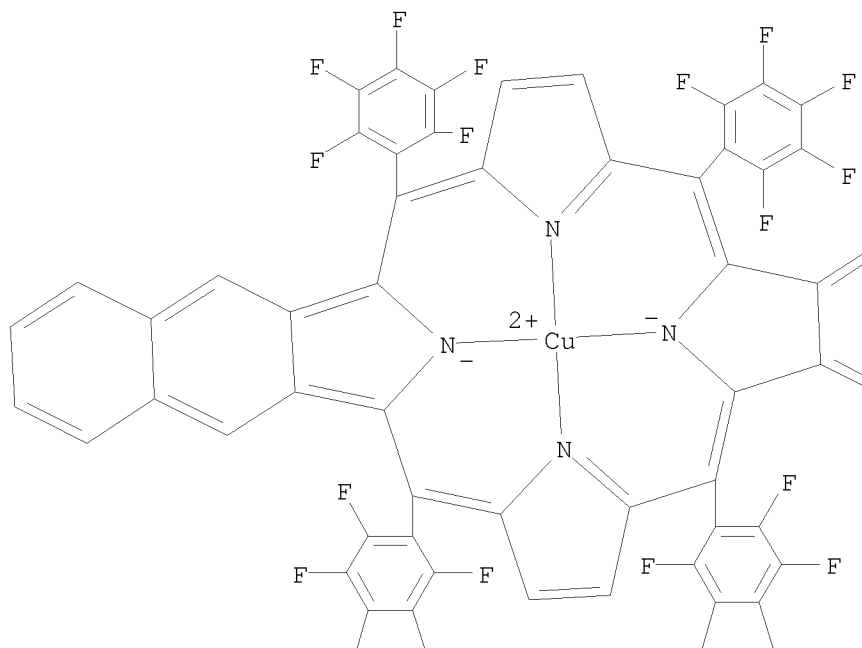


RN 401512-05-8 CAPLUS  
 CN Copper, [7,12,17,22-tetraphenyl-25H,27H-naphtho[2,3-b]porphinato(2-)-  
 κN25,κN26,κN27,κN28]-, (SP-4-1)- (9CI) (CA INDEX  
 NAME)

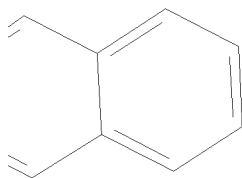


RN 401512-06-9 CAPLUS  
 CN Copper, [7,12,17,22-tetrakis(pentafluorophenyl)-25H,27H-naphtho[2,3-  
 b]porphinato(2-)-κN25,κN26,κN27,κN28]-, (SP-4-1)-  
 (9CI) (CA INDEX NAME)

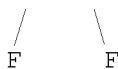
PAGE 1-A



PAGE 1-B



PAGE 2-A



REFERENCE COUNT:

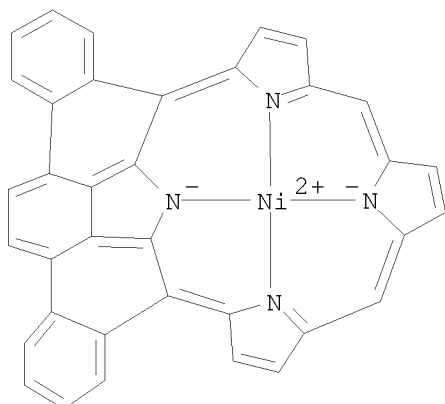
70

THERE ARE 70 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

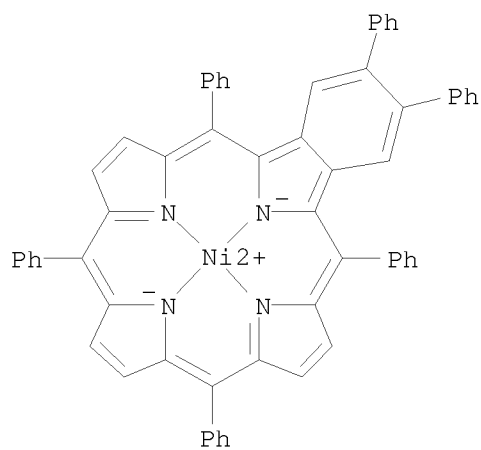
L9 ANSWER 41 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2001:733732 CAPLUS  
 DOCUMENT NUMBER: 136:47499  
 TITLE: Multicarbocycle formation mediated by arenoporphyrin  
 1,4-diradicals: Synthesis of picenoporphyrins  
 AUTHOR(S): Aihara, Hidenori; Jaquinod, Laurent; Nurco, Daniel J.;  
 Smith, Kevin M.  
 CORPORATE SOURCE: Dep. of Chemistry, University of California, Davis,  
 CA, 95616, USA  
 SOURCE: Angewandte Chemie, International Edition (2001),  
 40(18), 3439-3441  
 CODEN: ACIEF5; ISSN: 1433-7851  
 PUBLISHER: Wiley-VCH Verlag GmbH  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 136:47499  
 GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB The authors report unprecedented multicarbocycle formation on the  
 porphyrin periphery by Bergman aromatization of vicinal  
 dialkynylporphyrins, to produce a new class of highly  $\pi$ -extended  
 porphyrins. Nickel(II) 2,3-dialkynyl-5,10,15,20-tetraphenylporphyrins (I;  
 R = TMS, H, Bu, Ph) were prepared by Pd0-catalyzed cross-coupling reactions  
 of nickel(II) 2,3-dibromo-5,10,15,20-tetraphenylporphyrin with the  
 corresponding alkynyl trimethylstannanes. Refluxing the nickel(II)  
 2,3-dialkynyl-5,10,15,20-tetraphenylporphyrins (I; R = H, Bu, Ph) in 5 %  
 1,4-cyclohexadiene/chlorobenzene solution gave (II; R = H, Bu, Ph). The new  
 porphyrins obtained from this reactions are named "picenoporphyrins."  
 Compound I (R = H) gave none of the corresponding picenoporphyrin. II (R =  
 H) was characterized by single crystal x-ray diffraction anal. and <sup>1</sup>H NMR.  
 IT 380447-54-1P  
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
 (preparation and crystal structure of)  
 RN 380447-54-1 CAPLUS  
 CN Nickel, [1,21[1',2']:4,6[1'',2'']-dibenzene-23H,25H-benzo[b]porphinato(2-)-  
 κN23,κN24,κN25,κN26]-, (SP-4-1)-(9CI) (CA INDEX  
 NAME)

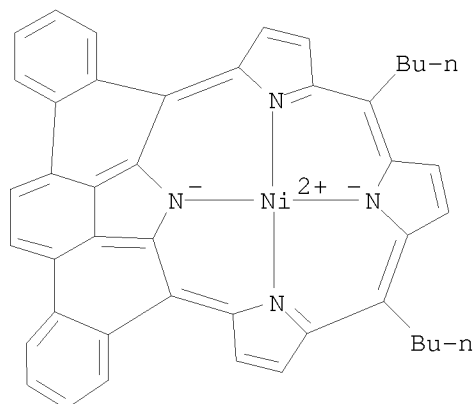


IT 740844-63-7P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation and crystal structure of)  
 RN 740844-63-7 CAPLUS  
 CN Nickel, [2,3,6,11,16,21-hexaphenyl-23H,25H-benzo[b]porphinato(2-)-  
 $\kappa$ N23, $\kappa$ N24, $\kappa$ N25, $\kappa$ N26]-, (SP-4-1)- (9CI) (CA INDEX  
 NAME)



IT 380447-56-3P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 RN 380447-56-3 CAPLUS  
 CN Nickel, [11,16-dibutyl-1,21[1',2']:4,6[1'',2'']-dibenzeno-23H,25H-  
 benzo[b]porphinato(2-)- $\kappa$ N23, $\kappa$ N24, $\kappa$ N25, $\kappa$ N26]-,  
 (SP-4-1)- (9CI) (CA INDEX NAME)





REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

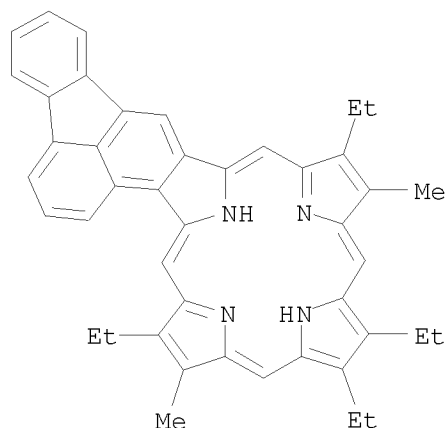
L9 ANSWER 42 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2001:253573 CAPLUS  
 DOCUMENT NUMBER: 135:33394  
 TITLE: Porphyrins with Exocyclic Rings. 16.1 Synthesis and Spectroscopic Characterization of Fluoranthoporphyrins, a New Class of Highly Conjugated Porphyrin Chromophores  
 AUTHOR(S): Lash, Timothy D.; Werner, Tonya M.; Thompson, Michelle L.; Manley, Jerad M.  
 CORPORATE SOURCE: Department of Chemistry, Illinois State University, Normal, IL, 61790-4160, USA  
 SOURCE: Journal of Organic Chemistry (2001), 66(9), 3152-3159  
 CODEN: JOCEAH; ISSN: 0022-3263  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 135:33394  
 GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

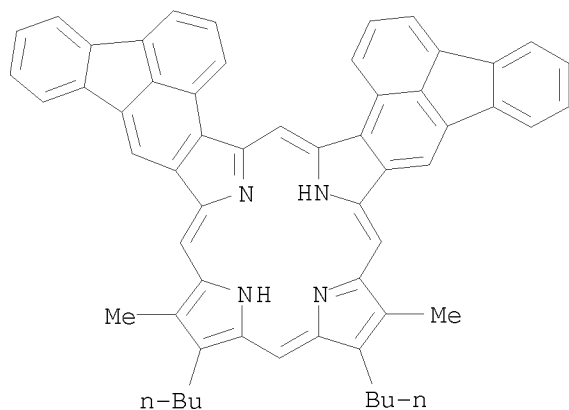
AB Porphyrins with fused aromatic rings are under detailed investigation due to their unique spectroscopic properties. To gain more insights into the effects due to ring annealation on the porphyrin chromophore, a series of fluoranthoporphyrins have been synthesized. Reaction of 3-nitrofluoranthene with isocyanoacetate esters in the presence of a phosphazene base afforded good yields of the fluorantho[2,3-c]pyrrole esters. Cleavage of the ester moiety with KOH in ethylene glycol afforded the parent heterocycle (I), and this condensed with 2 equiv of acetoxymethylpyrroles in refluxing acetic acid-2-propanol to afford tripyrranes. Following cleavage of the tert-Bu ester protective groups with TFA, "3 + 1" condensation with pyrrole dialdehyde gave the fluoranthoporphyrins (II) in good overall yields. In addition, reaction of tripyrrane with acenaphthopyrrole dialdehyde gave the mixed

acenaphthofluoranthoporphyrin (III) in excellent yields. A difluoranthoporphyrin (IV) was also prepared via a "2 + 2" MacDonald condensation. Reaction of fluoranthopyrrole with dimethoxymethane in the presence of p-toluenesulfonic acid gave the sym. dipyrromethane, and following ester saponification, this was condensed with a dipyrromethane dialdehyde to afford IV. The UV-vis spectra for these fluoranthoporphyrins gave a series of three broadened absorptions in the Soret band region, although the Q-bands were little effected by ring fusion. The nickel(II), copper(II), and zinc chelates were more unusual, showing strong absorptions near 600 nm. IV showed many of the same spectroscopic features, although the presence of two ring fusions gave rise to an increase in the spectroscopic shifts. III gave spectra that showed larger red shifts due to the acenaphthylene unit combined with the features due to the fluoranthene rings. This work further demonstrates the utility of aromatic ring fusion in altering the properties of porphyrinoid systems.

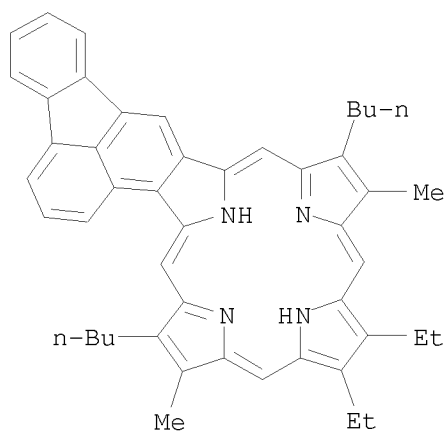
IT 343922-03-2P 343922-05-4P 343922-10-1P  
 RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (synthesis and spectroscopic characterization of fluoranthoporphyrins, a new class of highly conjugated porphyrin chromophores)  
 RN 343922-03-2 CAPLUS  
 CN 27H,29H-Fluorantheno[2,3-b]porphine,  
 12,17,18,23-tetraethyl-13,22-dimethyl- (9CI) (CA INDEX NAME)



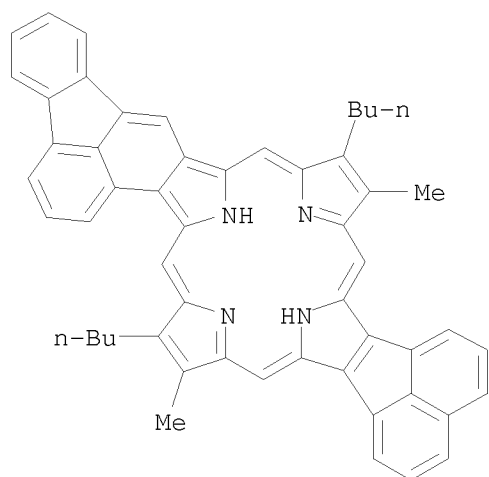
RN 343922-05-4 CAPLUS  
 CN 33H,35H-Difluorantheno[2,3-b:3',2'-g]porphine,  
 10,14-dibutyl-9,15-dimethyl- (9CI) (CA INDEX NAME)



RN 343922-10-1 CAPLUS  
 CN 27H,29H-Fluorantheno[2,3-b]porphine,  
 12,23-dibutyl-17,18-diethyl-13,22-dimethyl- (9CI) (CA INDEX NAME)

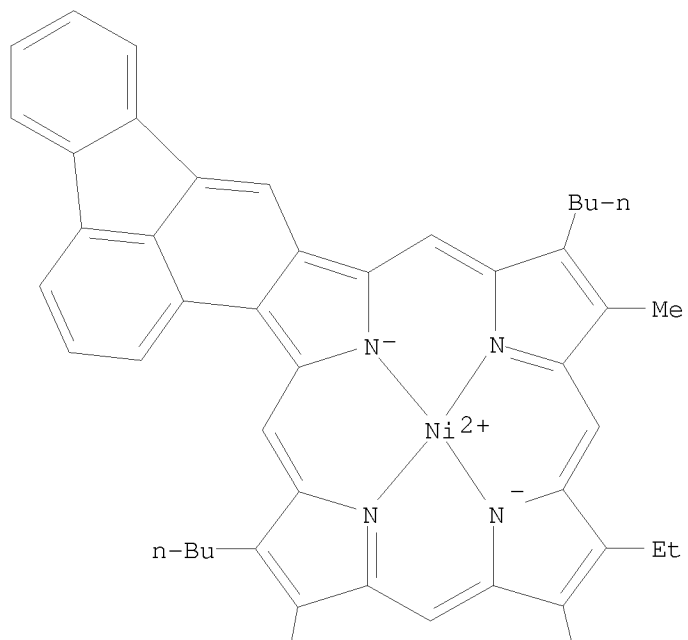


IT 343922-04-3P 344346-14-1P 344346-15-2P  
 344346-16-3P 344346-17-4P  
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
 (synthesis and spectroscopic characterization of fluoranthoporphyrins,  
 a new class of highly conjugated porphyrin chromophores)  
 RN 343922-04-3 CAPLUS  
 CN 31H,33H-Acenaphtho[1,2-b]fluorantheno[2,3-l]porphine,  
 12,27-dibutyl-13,26-dimethyl- (9CI) (CA INDEX NAME)



RN 344346-14-1 CAPLUS  
 CN Nickel, [12,23-dibutyl-17,18-diethyl-13,22-dimethyl-27H,29H-fluorantheno[2,3-b]porphinato(2-)-  
 $\kappa\text{N}27,\kappa\text{N}28,\kappa\text{N}29,\kappa\text{N}30$ ]-, (SP-4-2)- (9CI) (CA INDEX  
 NAME)

PAGE 1-A

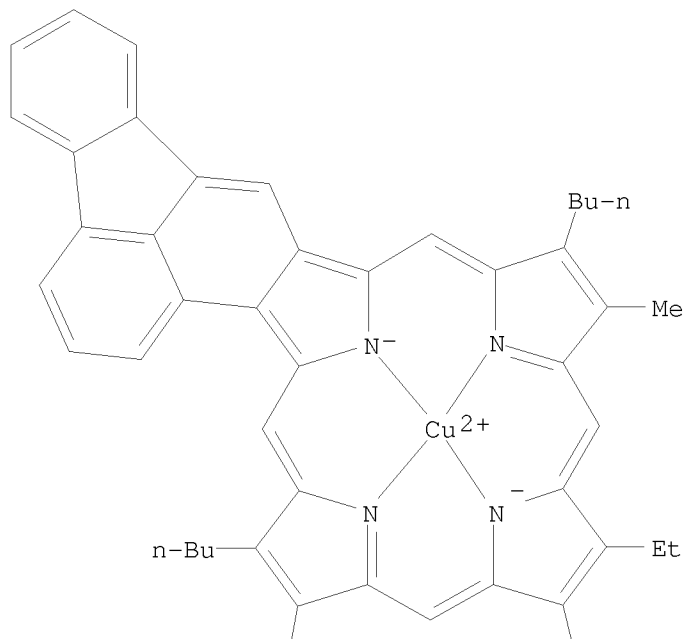


PAGE 2-A



RN 344346-15-2 CAPLUS  
 CN Copper, [12,23-dibutyl-17,18-diethyl-13,22-dimethyl-27H,29H-fluorantheno[2,3-b]porphinato(2-)-κN27,κN28,κN29,κN30]-, (SP-4-2)- (9CI) (CA INDEX NAME)

PAGE 1-A

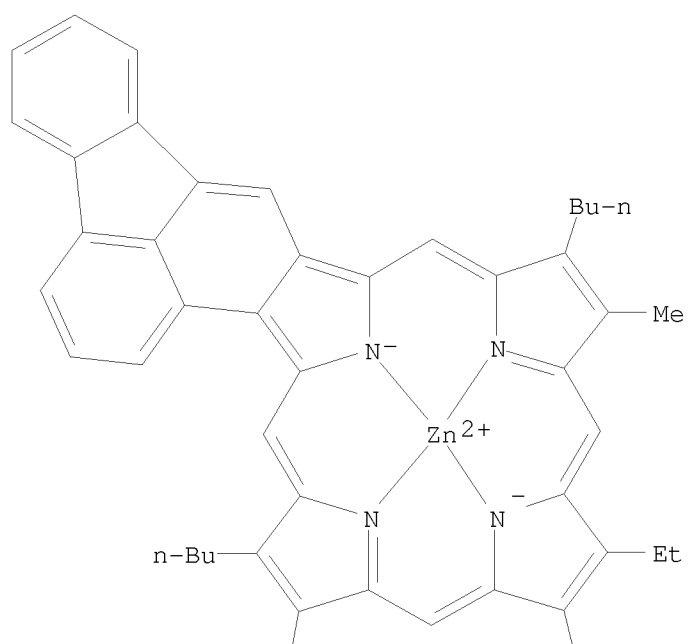


PAGE 2-A



RN 344346-16-3 CAPLUS  
 CN Zinc, [12,23-dibutyl-17,18-diethyl-13,22-dimethyl-27H,29H-fluorantheno[2,3-b]porphinato(2-)-κN27,κN28,κN29,κN30]-, (SP-4-2)- (9CI) (CA INDEX NAME)

PAGE 1-A

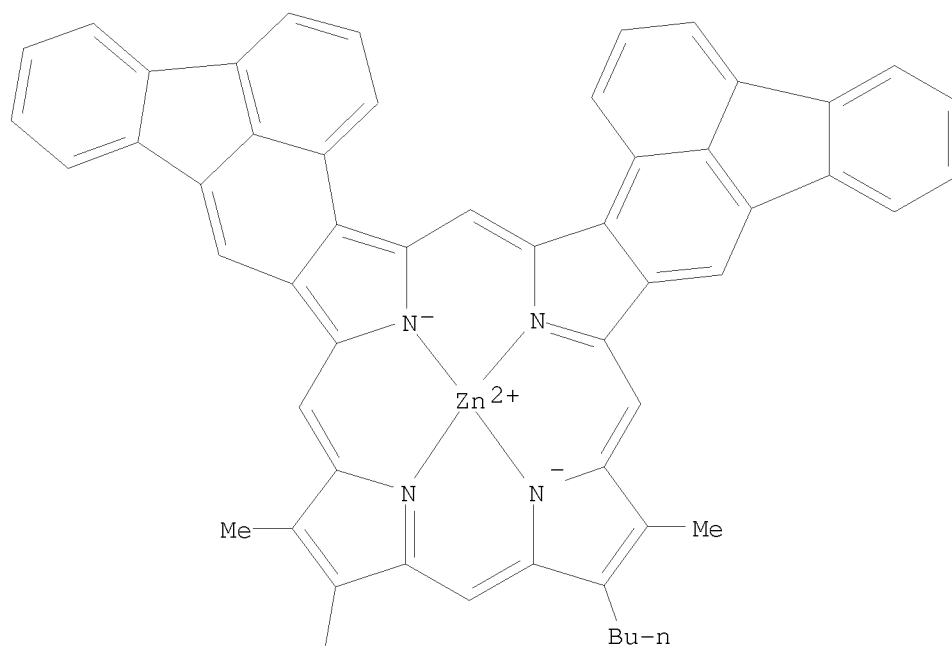


PAGE 2-A



RN 344346-17-4 CAPLUS  
 CN Zinc, [10,14-dibutyl-9,15-dimethyl-33H,35H-difluorantheno[2,3-b:3',2'-  
 g]porphinato(2-)-κN33,κN34,κN35,κN36]-, (SP-4-1)-  
 (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A

/  
n-Bu

REFERENCE COUNT: 64 THERE ARE 64 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 43 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2001:190573 CAPLUS  
 DOCUMENT NUMBER: 135:67922  
 TITLE: Molecular orbitals and electronic spectra of benzo-fused and related porphyrin analogues  
 AUTHOR(S): Kobayashi, Nagao; Konami, Hideo  
 CORPORATE SOURCE: Department of Chemistry, Graduate School of Science, Tohoku University, Sendai, 980-8578, Japan  
 SOURCE: Journal of Porphyrins and Phthalocyanines (2001), 5(3), 233-255  
 CODEN: JPPHFZ; ISSN: 1088-4246  
 PUBLISHER: John Wiley & Sons Ltd.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB MO calcns. of >60 porphyrinic  $\pi$  conjugated structures were performed within the framework of the PPP approximation The results of compds. are introduced and summarized to show how they vary depending on the systematic change in mol. structure. These are shown schematically or itemized. The authors' results are compared with the spectra of the

corresponding known compds. and with the MO results reported by previous workers, if available. In addition, the results have continually been compared, where possible, with those of tetraazaporphyrin or phthalocyanine systems. In naphthalene- or anthracene-fused compds., these mol.-centered orbitals often appear, and these are indicated using either triangles or circles in figures if they appear between HOMO - 3 and LUMO + 3 orbitals.

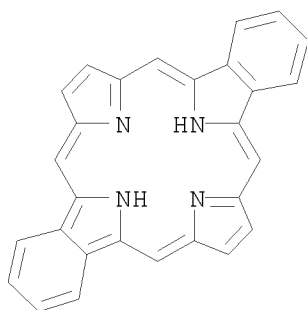
IT 36547-73-6, 25H,27H-Dibenzo[b,l]porphine 194869-07-3,  
29H,31H-Dinaphtho[2,3-b:2',3'-l]porphine 227204-77-5,  
33H,35H-Dianthra[2,3-b:2',3'-l]porphine 345906-82-3  
345906-83-4 345906-84-5 345906-88-9  
345906-89-0 345906-90-3 345906-94-7  
345906-95-8 345906-96-9 345907-09-7,  
28H,30H-Tribenzo[b,g,l]porphine 345907-14-4

RL: PRP (Properties)

(mol. orbitals and electronic spectra of benzo-fused and related porphyrin analogs)

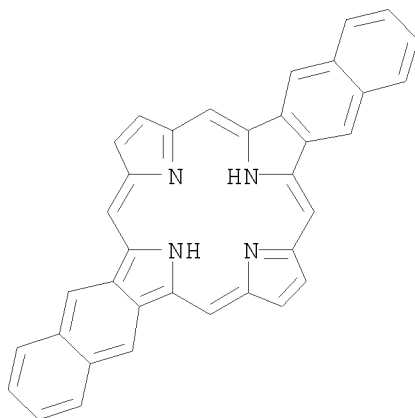
RN 36547-73-6 CAPLUS

CN 25H,27H-Dibenzo[b,l]porphine (9CI) (CA INDEX NAME)



RN 194869-07-3 CAPLUS

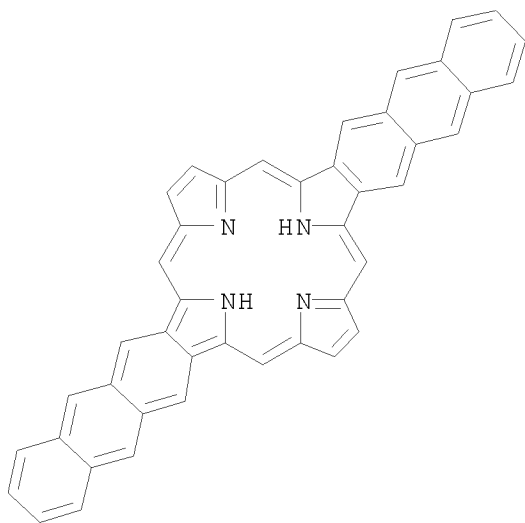
CN 29H,31H-Dinaphtho[2,3-b:2',3'-l]porphine (9CI) (CA INDEX NAME)



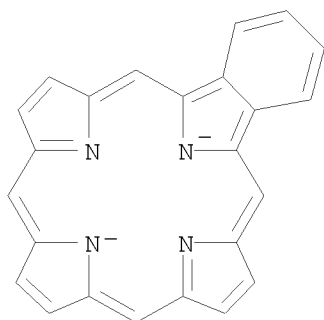
RN 227204-77-5 CAPLUS

CN 33H,35H-Dianthra[2,3-b:2',3'-l]porphine (9CI) (CA INDEX NAME)

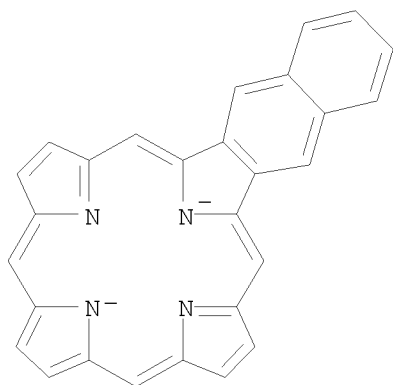




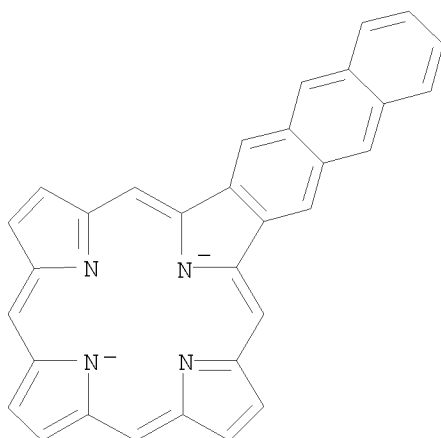
RN 345906-82-3 CAPLUS  
 CN 23H,25H-Benzo[b]porphine, ion(2-) (9CI) (CA INDEX NAME)



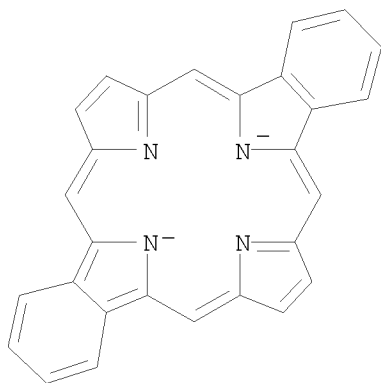
RN 345906-83-4 CAPLUS  
 CN 25H,27H-Naphtho[2,3-b]porphine, ion(2-) (9CI) (CA INDEX NAME)



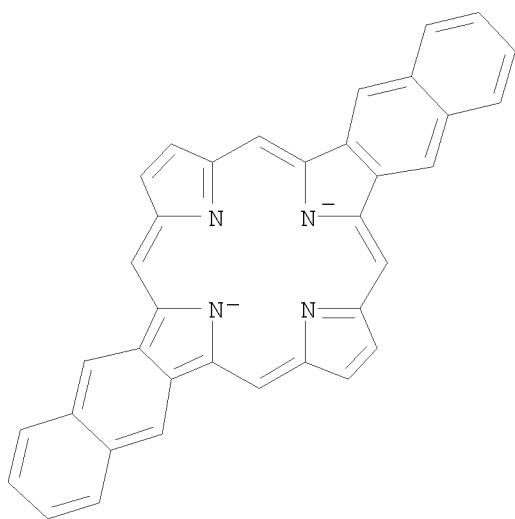
RN 345906-84-5 CAPLUS  
 CN 27H,29H-Anthra[2,3-b]porphine, ion(2-) (9CI) (CA INDEX NAME)



RN 345906-88-9 CAPLUS  
 CN 25H,27H-Dibenzo[b,1]porphine, ion(2-) (9CI) (CA INDEX NAME)

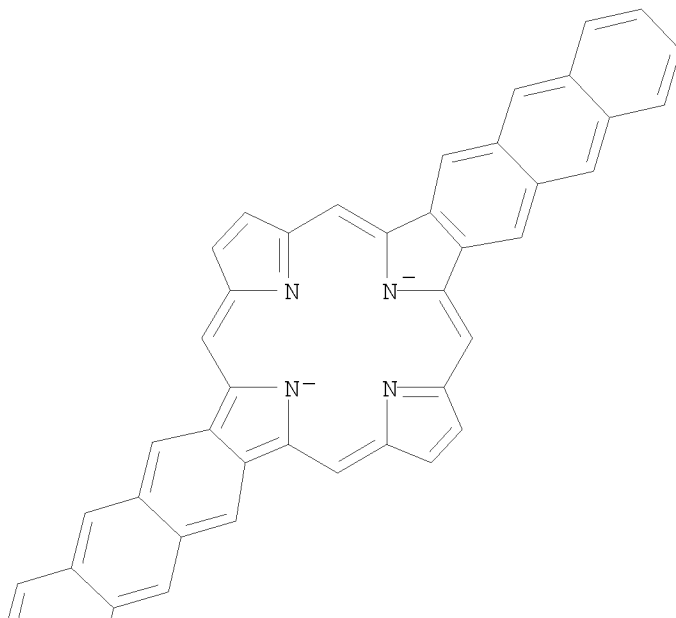


RN 345906-89-0 CAPLUS  
CN 29H,31H-Dinaphtho[2,3-b:2',3'-l]porphine, ion(2-) (9CI) (CA INDEX NAME)

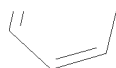


RN 345906-90-3 CAPLUS  
CN 33H,35H-Dianthra[2,3-b:2',3'-l]porphine, ion(2-) (9CI) (CA INDEX NAME)

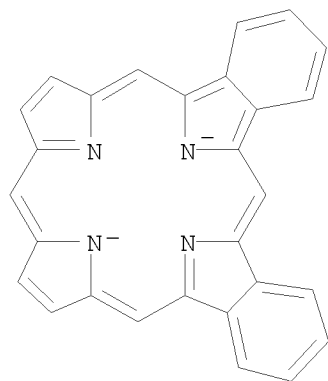
PAGE 1-A



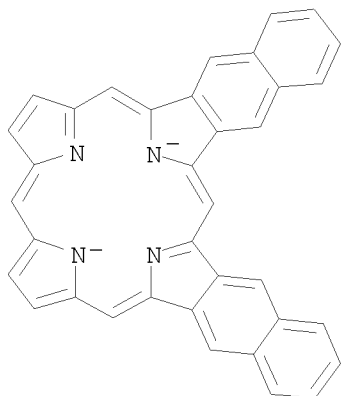
PAGE 2-A



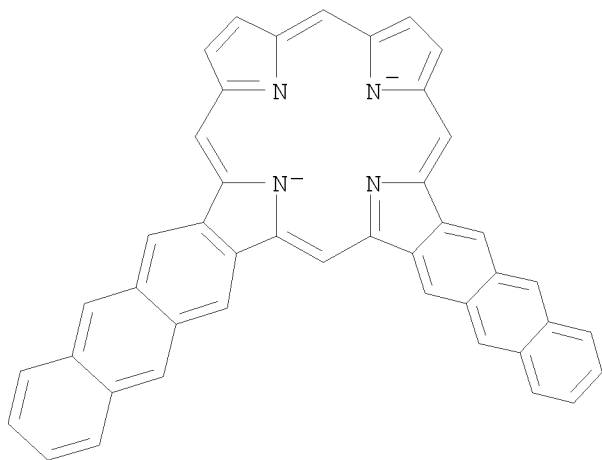
RN 345906-94-7 CAPLUS  
CN 25H,27H-Dibenzo[b,g]porphine, ion(2-) (9CI) (CA INDEX NAME)



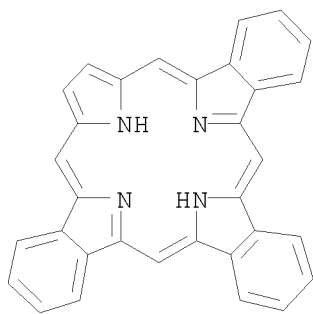
RN 345906-95-8 CAPLUS  
CN 29H,31H-Dinaphtho[2,3-b:2',3'-g]porphine, ion(2-) (9CI) (CA INDEX NAME)



RN 345906-96-9 CAPLUS  
 CN 33H,35H-Dianthra[2,3-b:2',3'-g]porphine, ion(2-) (9CI) (CA INDEX NAME)



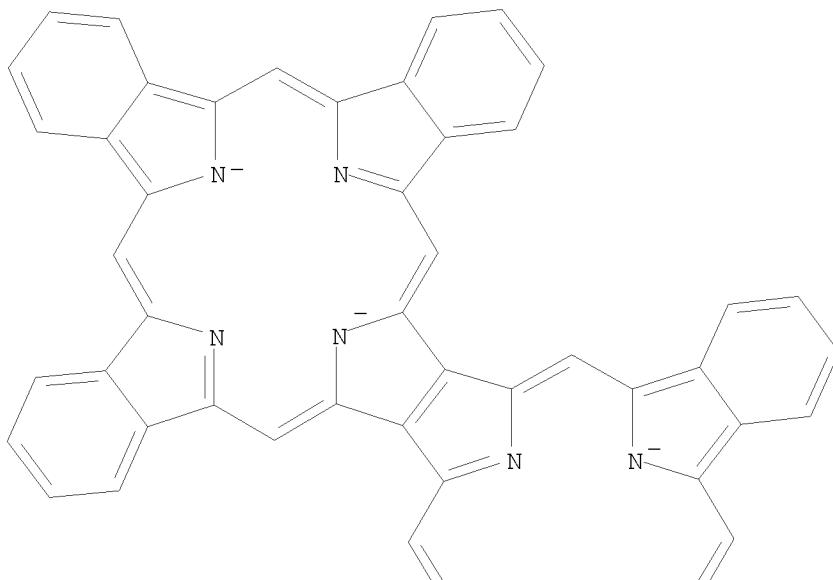
RN 345907-09-7 CAPLUS  
 CN 28H,30H-Tribenzo[b,g,l]porphine (9CI) (CA INDEX NAME)



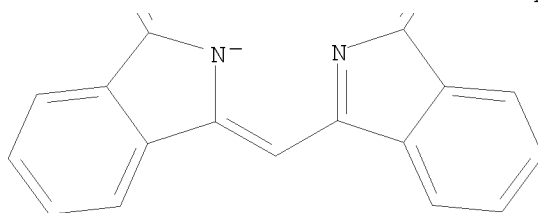
RN 345907-14-4 CAPLUS

CN 49H,51H,53H,55H-Tribenzo[b,g,l]tribenzo[7,8:12,13:17,18]porphino[2,3-q]porphine, ion(4-) (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



REFERENCE COUNT: 62 THERE ARE 62 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 44 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2000:742739 CAPLUS  
 DOCUMENT NUMBER: 134:42009  
 TITLE: Porphyrins with Exocyclic Rings. 15.1 Synthesis of Quino- and Isoquinoporphyrins, Aza Analogues of the Naphthoporphyrins  
 AUTHOR(S): Lash, Timothy D.; Gandhi, Virajkumar  
 CORPORATE SOURCE: Department of Chemistry, Illinois State University, Normal, IL, 61790-4160, USA  
 SOURCE: Journal of Organic Chemistry (2000), 65(23), 8020-8026  
 CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 134:42009

AB Porphyrins with fused isoquinoline and quinoline units have been prepared by the "3 + 1" methodol. 5-Nitroisoquinoline and 6-nitroquinoline condensed with Et isocyanoacetate in the presence of a phosphazene base to give isoquino- and quinopyrroles, resp. Ester saponification and decarboxylation with

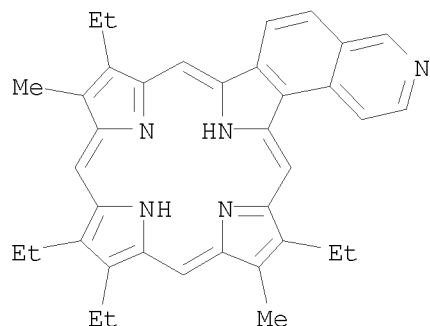
KOH in ethylene glycol at 190 °C gave the parent azatricycles, and these were further condensed with 2 equiv of an acetoxymethylpyrrole to give the corresponding tripyrranes protected at the terminal positions as their tert-Bu esters. In a one-pot procedure, the ester protective groups were cleaved with TFA, and following dilution with dichloromethane, "3 + 1" condensation with a pyrrole dialdehyde and dehydrogenation of the phlorin intermediate with DDQ gave the targeted azanaphthoporphyrins in excellent yields. Although the UV-vis spectra of these new porphyrin systems are unexceptional, they show promise for further functionalization and applications in the development of porphyrin arrays. In addition, a zinc chelate of the isoquinoporphyrin system shows a high degree of regioselective intermol. interaction/aggregation in chloroform solution that may lead to selectivity in mol. recognition studies.

IT 312273-72-6P 312273-73-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (synthesis of quino- and isoquinoporphyrins, aza analogs of the naphthoporphyrins)

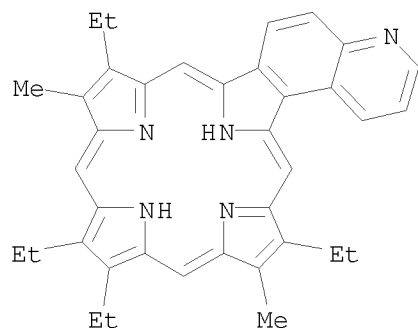
RN 312273-72-6 CAPLUS

CN 25H,27H-Isoquino[5,6-b]porphine, 10,15,16,21-tetraethyl-11,20-dimethyl- (9CI) (CA INDEX NAME)

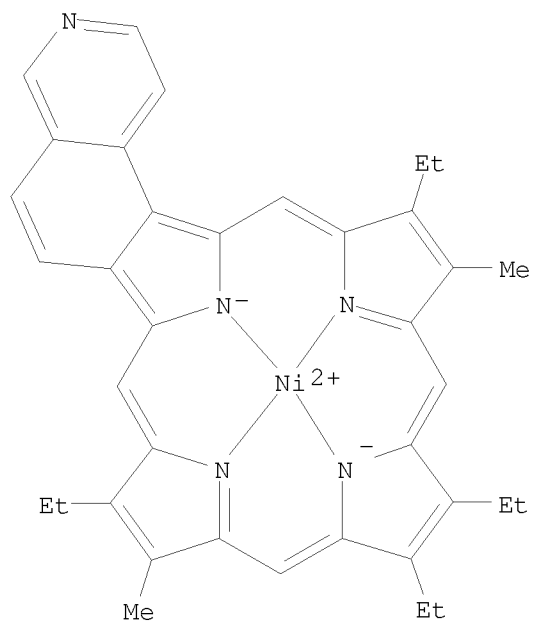


RN 312273-73-7 CAPLUS

CN 25H,27H-Quino[5,6-b]porphine, 10,15,16,21-tetraethyl-11,20-dimethyl- (CA INDEX NAME)

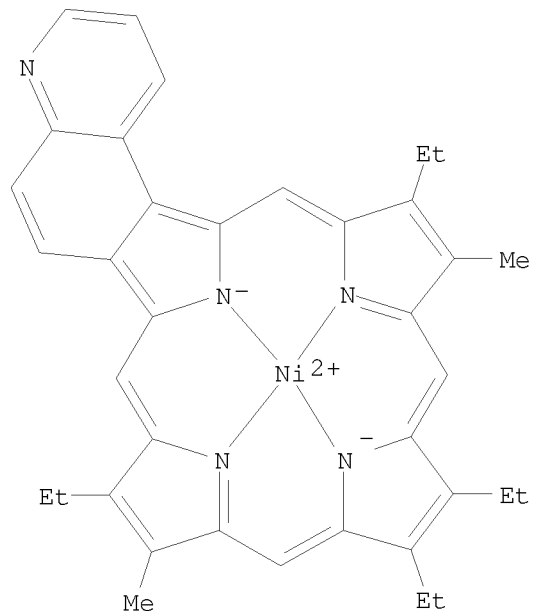


IT 312636-80-9P 312636-81-0P 312636-82-1P  
 312636-83-2P 312636-84-3P 312636-85-4P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (synthesis of quino- and isoquinoporphyrins, aza analogs of the  
 naphthoporphyrins)  
 RN 312636-80-9 CAPLUS  
 CN Nickel, [10,15,16,21-tetraethyl-11,20-dimethyl-25H,27H-isoquino[5,6-  
 b]porphinato(2-)-κN25,κN26,κN27,κN28]-, (SP-4-2)-  
 (9CI) (CA INDEX NAME)

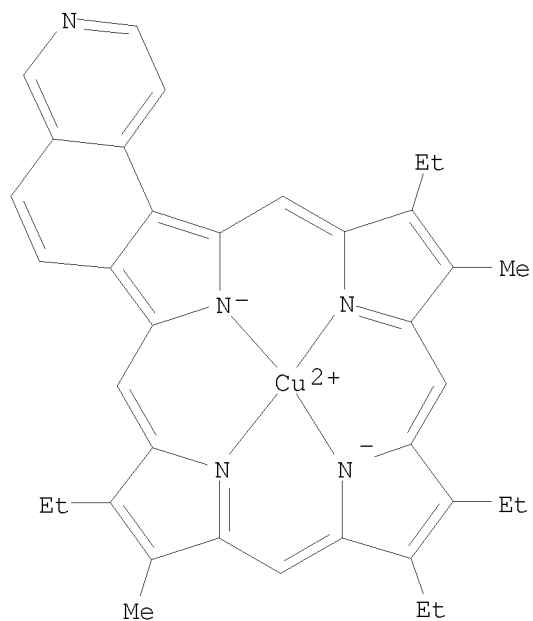


RN 312636-81-0 CAPLUS  
 CN Nickel, [10,15,16,21-tetraethyl-11,20-dimethyl-25H,27H-quino[5,6-  
 b]porphinato(2-)-κN25,κN26,κN27,κN28]-, (SP-4-2)-  
 (9CI) (CA INDEX NAME)



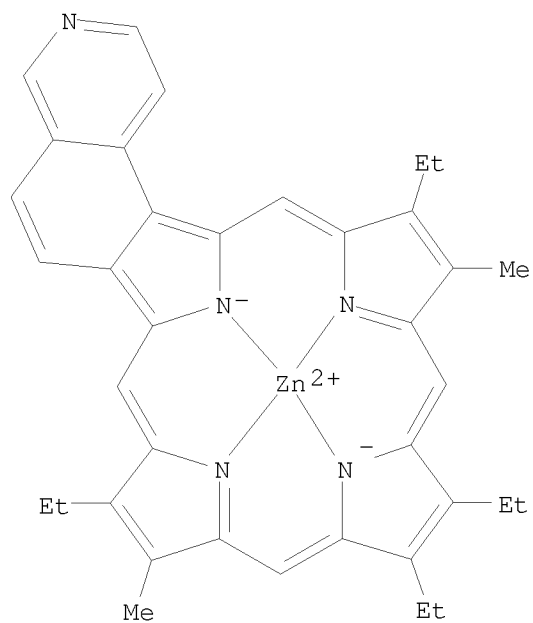


RN 312636-82-1 CAPLUS  
 CN Copper, [10,15,16,21-tetraethyl-11,20-dimethyl-25H,27H-isoquino[5,6-b]porphinato(2-)-κN25,κN26,κN27,κN28]-, (SP-4-2)-(9CI) (CA INDEX NAME)



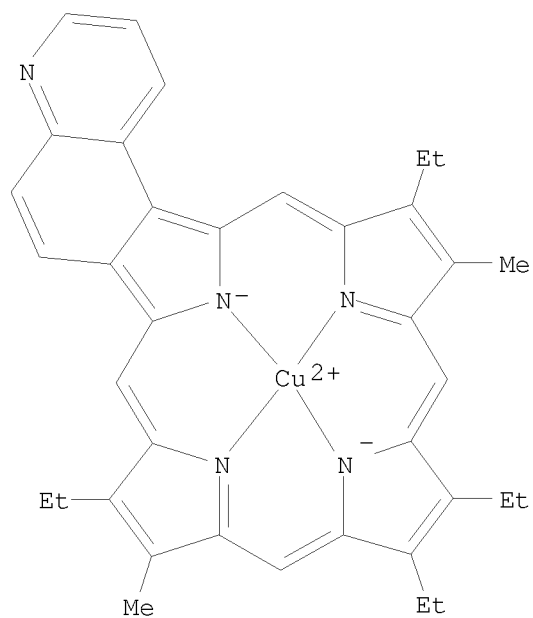
RN 312636-83-2 CAPLUS  
 CN Zinc, [10,15,16,21-tetraethyl-11,20-dimethyl-25H,27H-isoquino[5,6-b]porphinato(2-)-κN25,κN26,κN27,κN28]-, (SP-4-2)-

(9CI) (CA INDEX NAME)



RN 312636-84-3 CAPLUS

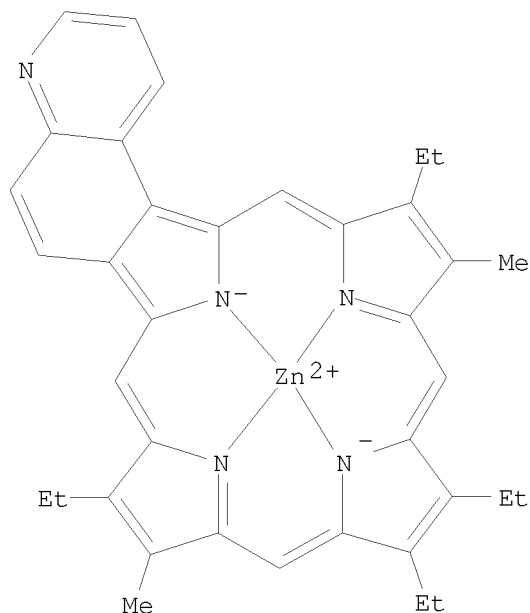
CN Copper, [10,15,16,21-tetraethyl-11,20-dimethyl-25H,27H-quino[5,6-b]porphinato(2-)-κN25,κN26,κN27,κN28]-, (SP-4-2)-  
(9CI) (CA INDEX NAME)



RN 312636-85-4 CAPLUS

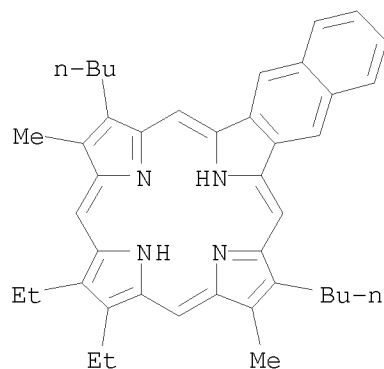
10583126.trn

CN Zinc, [10,15,16,21-tetraethyl-11,20-dimethyl-25H,27H-quinol[5,6-b]porphinato(2-)-κN25,κN26,κN27,κN28]-, (SP-4-2)-  
(9CI) (CA INDEX NAME)



REFERENCE COUNT: 88 THERE ARE 88 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 45 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2000:350663 CAPLUS  
 DOCUMENT NUMBER: 133:150401  
 TITLE: A new synthesis of [2,3]naphthoporphyrins  
 AUTHOR(S): Ito, Satoshi; Ochi, Naoyuki; Murashima, Takashi; Ono, Noboru; Uno, Hidemitsu  
 CORPORATE SOURCE: Dep. Chem., Fac. Sci., Ehime University, Matsuyama, Japan  
 SOURCE: Chemical Communications (Cambridge) (2000), (11), 893-894  
 CODEN: CHCOFS; ISSN: 1359-7345  
 PUBLISHER: Royal Society of Chemistry  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 133:150401  
 AB A new synthesis of [2,3]naphthoporphyrins using 4,9-ethano-2H-benz[f]isoindole as a synthon of 2H-benz[f]isoindole is described; soluble precursors of [2,3]naphthoporphyrins are converted into insol. [2,3]naphthoporphyrins by simply heating at 290 °C.  
 IT 287378-42-1P  
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (synthesis and UV-VIS data of naphthoporphyrins)  
 RN 287378-42-1 CAPLUS  
 CN 25H,27H-Naphtho[2,3-b]porphine, 9,20-dibutyl-14,15-diethyl-10,19-dimethyl-  
 (9CI) (CA INDEX NAME)



REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 46 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2000:298635 CAPLUS

DOCUMENT NUMBER: 132:339834

TITLE: Distortion and aromatization factors on the complexing ability of tetrapyrrole macrocycles in acetonitrile  
AUTHOR(S): Berezin, D. B.; Bazlova, I. Yu.; Malkova, O. V.; Andrianov, V. G.

CORPORATE SOURCE: Ivanovo State Academy of Chemical Technology, Ivanovo, Russia

SOURCE: Russian Journal of Coordination Chemistry (Translation of Koordinatsionnaya Khimiya) (2000), 26(4), 295-299  
CODEN: RJCCEY; ISSN: 1070-3284

PUBLISHER: MAIK Nauka/Interperiodica Publishing

DOCUMENT TYPE: Journal

LANGUAGE: English

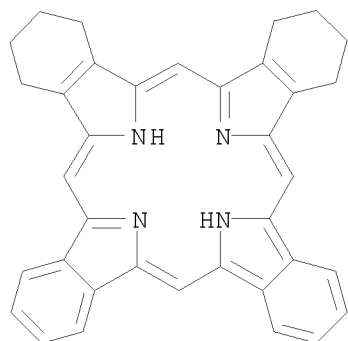
AB The kinetics of complexation between porphyrins and zinc acetate in acetonitrile was studied for the porphyrins belonging to various structural groups, including aza-, benzo-, and distorted N- and multiply substituted macrocycles. The effects of the distortion, on the one hand, and the enhanced rigidity of a macrocycle, on the other, on the complexation process were considered. The coordination of the distorted porphyrins to metal salts is facilitated because of the disturbance of the steric component of the macrocyclic effect (MCE), whereas the complexation of the rigid macrocycles is facilitated because of the activation of the electronic component of MCE.

IT 267889-11-2

RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)  
(distortion and aromatization factors on complexing ability of tetrapyrrole macrocycles in acetonitrile)

RN 267889-11-2 CAPLUS

CN 29H,31H-Tetrabenzo[b,g,l,q]porphine, 1,2,3,4,8,9,10,11-octahydro- (9CI)  
(CA INDEX NAME)



REFERENCE COUNT: 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 47 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2000:261510 CAPLUS

DOCUMENT NUMBER: 132:356110

TITLE: Diels-alder reaction of Ni(II)

$\beta$ -vinyl-meso-tetraphenylporphyrin; a general method for synthesis of functionalized porphyrins

AUTHOR(S): Matsumoto, Kiyoshi; Kimura, Shinya; Morishita, Takuya; Misumi, Yukihiro; Hayashi, Naoto

CORPORATE SOURCE: Graduate School of Human and Environmental Studies, Kyoto University, Kyoto, 606-8501, Japan

SOURCE: Synlett (2000), (2), 233-235  
CODEN: SYNLES; ISSN: 0936-5214

PUBLISHER: Georg Thieme Verlag

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Ni(II)  $\beta$ -vinyl-meso-tetraphenylporphyrin underwent Diels-Alder reaction with a variety of dienophiles to give the corresponding porphyrins via 1,3-H shift of the initial adducts in good to moderate yields.

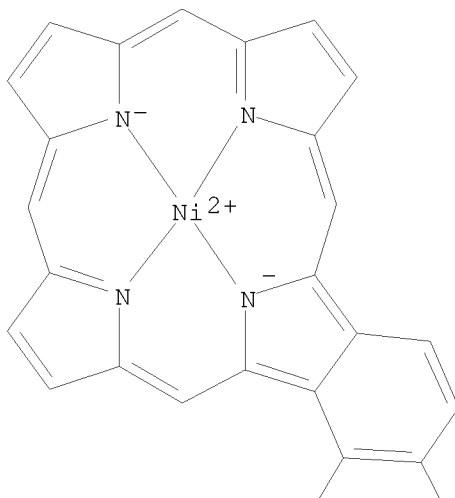
IT 269081-30-3P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation by Diels Alder reaction of Ni(II)  
 $\beta$ -vinyl-meso-tetraphenylporphyrin with dienophiles)

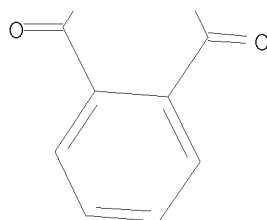
RN 269081-30-3 CAPLUS

CN Nickel, [27H,29H-anthra[1,2-b]porphine-21,26-dionato(2-)-  
 $\kappa N27, \kappa N28, \kappa N29, \kappa N30$ ]-, (SP-4-2)- (9CI) (CA INDEX  
NAME)

PAGE 1-A



PAGE 2-A



REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 48 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2000:26820 CAPLUS

DOCUMENT NUMBER: 132:207689

TITLE: A new synthesis of benzoporphyrins using 4,7-dihydro-4,7-ethano-2H-isoindole as an isoindole equivalent

AUTHOR(S): Ito, Satoshi; Ochi, Naoyuki; Murashima, Takashi; Uno, Hidemitsu; Ono, Noboru

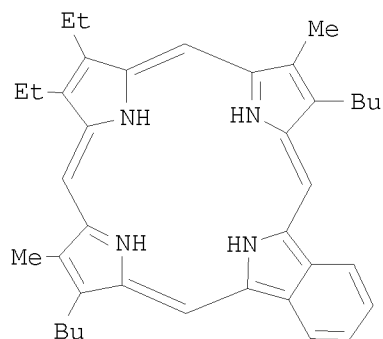
CORPORATE SOURCE: Department of Chemistry, Faculty of Science, Ehime University, Matsuyama, 790-8577, Japan

SOURCE: Heterocycles (2000), 52(1), 399-411

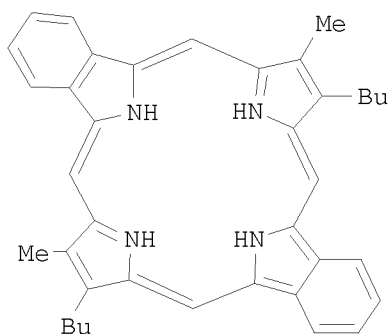
CODEN: HETCYAM; ISSN: 0385-5414

PUBLISHER: Japan Institute of Heterocyclic Chemistry

DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 132:207689  
 GI



I



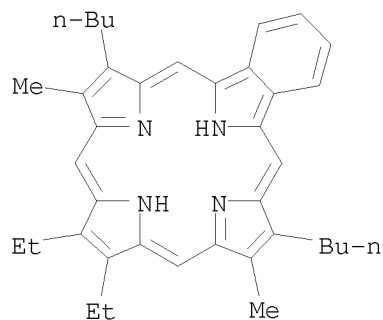
II

AB Various benzoporphyrins and their metal complexes were obtained in 100% yield by heating porphyrins fused with bicyclo[2.2.2]octadiene at 200°C. This thermal (retro Diels-Alder) reaction proceeds very cleanly to give pure monobenzoporphyrins (e.g., I) and dibenzoporphyrins (e.g., II) without further purification

IT 213920-98-0P 260250-70-2P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (synthesis of benzoporphyrins using 4,7-dihydro-4,7-ethano-2H-isoindole as an isoindole equivalent)

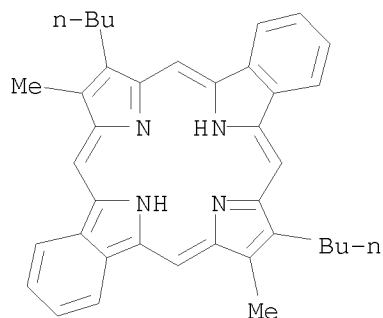
RN 213920-98-0 CAPLUS

CN 23H,25H-Benzo[b]porphine, 8,19-dibutyl-13,14-diethyl-9,18-dimethyl- (9CI)  
 (CA INDEX NAME)



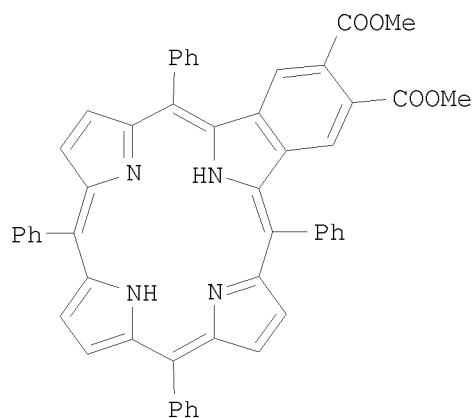
RN 260250-70-2 CAPLUS

CN 25H,27H-Dibenzo[b,1]porphine, 8,21-dibutyl-9,20-dimethyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 49 THERE ARE 49 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 49 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1999:777601 CAPLUS  
 DOCUMENT NUMBER: 132:116635  
 TITLE: Synthesis and chemistry of new benzoporphyrins  
 AUTHOR(S): Graca, M.; Vicente, H.; Jaquinod, Laurent; Khoury, Richard G.; Madrona, Acacia Y.; Smith, Kevin M.  
 CORPORATE SOURCE: Department of Chemistry, University of California, Davis, CA, 95616, USA  
 SOURCE: Tetrahedron Letters (1999), 40(50), 8763-8766  
 CODEN: TELEAY; ISSN: 0040-4039  
 PUBLISHER: Elsevier Science Ltd.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



I

AB ML (H<sub>2</sub>L = I) are the major products obtained from the cycloaddn. reactions of ML1 (M = Cu, Ni; H<sub>2</sub>L1 = 5,10,15,20-tetraphenylpyrrolo[3,4-b]porphine) with di-Me acetylenedicarboxylate. In the presence of excess dienophile a bis-adduct is also obtained which undergoes retro-Diels-Alder reaction to produce CuL. CuL was converted into the 1st reported  $\beta$ -fused benzochlorins and the free-base benzoporphyrin I was regioselectively and



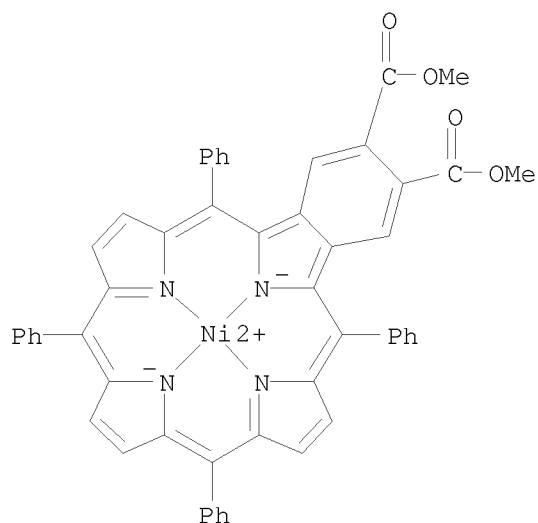
exhaustively brominated.

IT 255366-66-6P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(preparation and crystal structure of)

RN 255366-66-6 CAPLUS

CN Nickel, [dimethyl 6,11,16,21-tetraphenyl-23H,25H-benzo[b]porphine-2,3-dicarboxylato(2-)- $\kappa$ N23, $\kappa$ N24, $\kappa$ N25, $\kappa$ N26]-, (SP-4-1)-  
(9CI) (CA INDEX NAME)

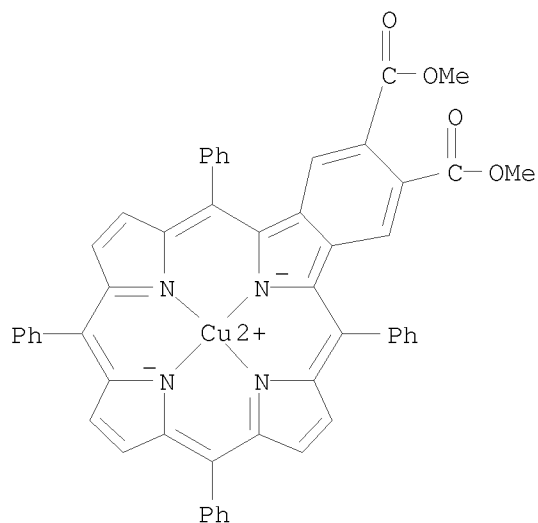


IT 255366-65-5P

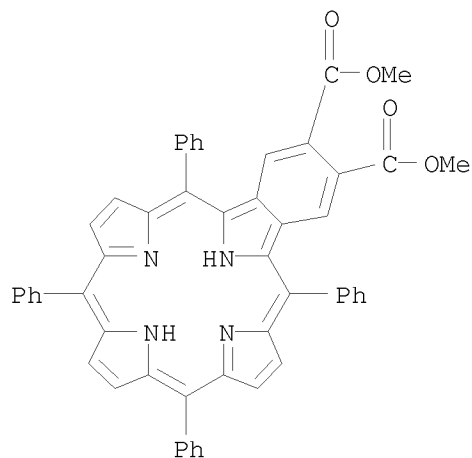
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(preparation and nitration and demetalation)

RN 255366-65-5 CAPLUS

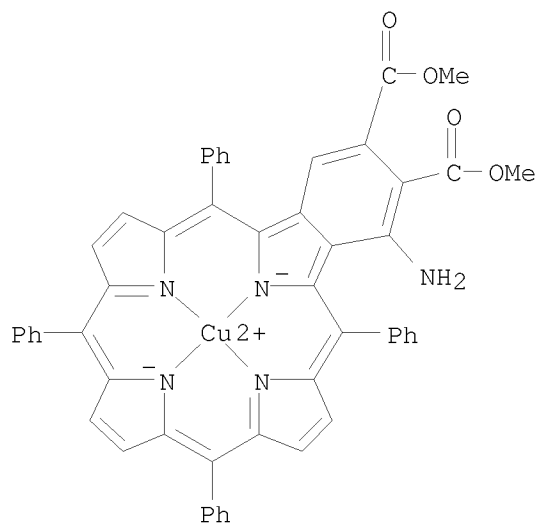
CN Copper, [dimethyl 6,11,16,21-tetraphenyl-23H,25H-benzo[b]porphine-2,3-dicarboxylato(2-)- $\kappa$ N23, $\kappa$ N24, $\kappa$ N25, $\kappa$ N26]-, (SP-4-1)-  
(9CI) (CA INDEX NAME)



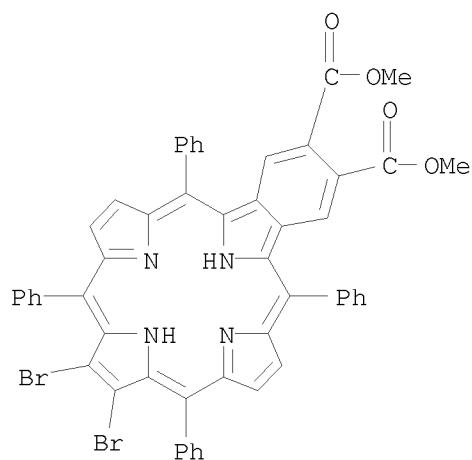
IT 255366-70-2P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (preparation and regioselective and exhaustive bromination)  
 RN 255366-70-2 CAPLUS  
 CN 23H,25H-Benzo[b]porphine-2,3-dicarboxylic acid, 6,11,16,21-tetraphenyl-,  
 dimethyl ester (9CI) (CA INDEX NAME)



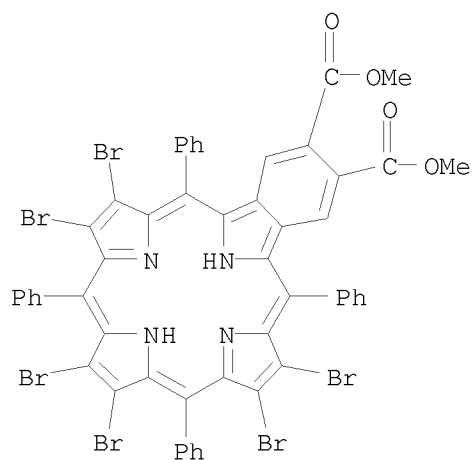
IT 255366-64-4P 255366-71-3P 255366-72-4P  
 255394-45-7P 255394-46-8P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 RN 255366-64-4 CAPLUS  
 CN Copper, [dimethyl 1-amino-6,11,16,21-tetraphenyl-23H,25H-benzo[b]porphine-  
 2,3-dicarboxylato(2-)-κN23,κN24,κN25,κN26]-,  
 (SP-4-2)- (9CI) (CA INDEX NAME)



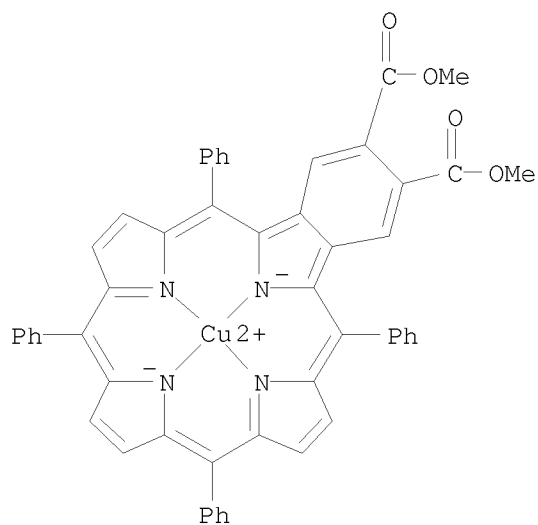
RN 255366-71-3 CAPLUS  
 CN 23H,25H-Benzo[b]porphine-2,3-dicarboxylic acid,  
 13,14-dibromo-6,11,16,21-tetraphenyl-, dimethyl ester (9CI) (CA INDEX  
 NAME)



RN 255366-72-4 CAPLUS  
 CN 23H,25H-Benzo[b]porphine-2,3-dicarboxylic acid,  
 8,9,13,14,18,19-hexabromo-6,11,16,21-tetraphenyl-, dimethyl ester (9CI)  
 (CA INDEX NAME)

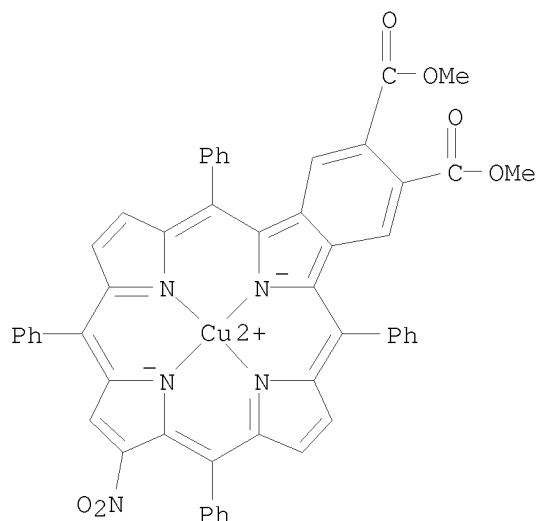


RN 255394-45-7 CAPLUS  
 CN Copper, [dimethyl 8(or 9)-nitro-6,11,16,21-tetraphenyl-23H,25H-benzo[b]porphine-2,3-dicarboxylato(2-)-κN23,κN24,κN25,κN26]- (9CI) (CA INDEX NAME)



D1-NO<sub>2</sub>

RN 255394-46-8 CAPLUS  
 CN Copper, [dimethyl 13-nitro-6,11,16,21-tetraphenyl-23H,25H-benzo[b]porphine-2,3-dicarboxylato(2-)-κN23,κN24,κN25,κN26]-, (SP-4-2)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

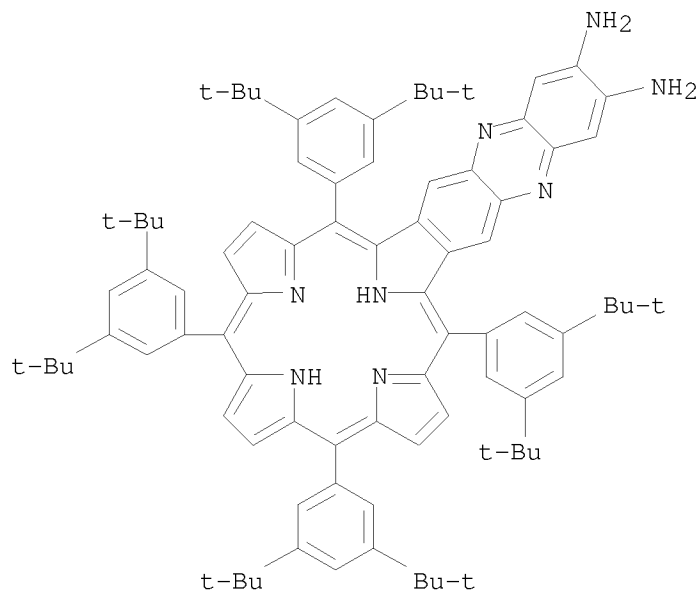
L9 ANSWER 50 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1999:505595 CAPLUS  
 DOCUMENT NUMBER: 131:280533  
 TITLE: Strict geometric control in metalated porphyrin-ligand supramolecular systems  
 AUTHOR(S): Schultz, Austin C.; Johnston, Martin R.; Warrenner, Ronald N.; Gunter, Maxwell J.  
 CORPORATE SOURCE: Centre for Molecular Architecture, Central Queensland University, Rockhampton, 4702, Australia  
 SOURCE: ECHET98: Electronic Conference on Heterocyclic Chemistry, June 29-July 24, 1998 (1998), 331-341. Editor(s): Rzepa, Henry S.; Kappe, C. Oliver; Leach, Christopher. Imperial College Press: London, UK. CODEN: 67TSA2  
 DOCUMENT TYPE: Conference; (computer optical disk)  
 LANGUAGE: English  
 GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB The cycloaddn. ligand delivery reagents 7,8-diazaphencyclone 9 and 3,6-di-(2'-pyridyl)-s-tetrazine 10, were reacted with pre-prepared porphyrin dienophiles, to obtain structurally organized porphyrin-ligand couples I-III. Central to this process was the synthesis of rigid alicyclic BLOCKs, which contained an  $\alpha$ -dione and a strained dienophilic  $\pi$ -center, thereby providing the ability to fuse the porphyrin (via porphyrin diamine) and ligand moieties (by cycloaddn.) site specifically onto the spacer framework.

IT 245445-24-3  
 RL: RCT (Reactant); RACT (Reactant or reagent)

(for preparation of porphyrin-ligand supramol. and its zinc complex)  
 RN 245445-24-3 CAPLUS  
 CN 27H,29H-Phenazino[2,3-b]porphine-2,3-diamine,  
 8,13,18,21-tetrakis[3,5-bis(1,1-dimethylethyl)phenyl]- (9CI) (CA INDEX  
 NAME)



REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 51 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1999:304475 CAPLUS  
 DOCUMENT NUMBER: 131:52446  
 TITLE: Rigid Fused Oligoporphyrins as Potential Versatile  
 Molecular Wires. 2. B3LYP and SCF Calculated Geometric  
 and Electronic Properties of 98 Oligoporphyrin and  
 Related Molecules  
 AUTHOR(S): Reimers, Jeffrey R.; Hall, Lachlan E.; Crossley,  
 Maxwell J.; Hush, Noel. S.  
 CORPORATE SOURCE: School of Chemistry and Department of Biochemistry,  
 University of Sydney, Sydney, NSW 2006, Australia  
 SOURCE: Journal of Physical Chemistry A (1999), 103(22),  
 4385-4397  
 CODEN: JPFAFH; ISSN: 1089-5639  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB To examine their basic operational principles and to explore synthetic  
 possibilities, the authors optimize the geometry of 85 oligoporphyrin and  
 related mols. including porphyrin dimers and trimers using the accurate  
 B3LYP d.-functional technique; Also, a scheme is developed by which  
 accurate geometries of oligoporphyrins of arbitrary size can be estimated, and  
 this is applied to determine the geometries of a further 13 porphyrin trimers  
 and tetramers. At these geometries the authors analyze SCF orbital

properties to determine the superexchange electronic couplings within the oligoporphyrins. Couplings were monitored for bridge-length dependence and interpreted in terms of a detailed description involving bridge-porphyrin orbital resonances, as well as in terms of a simpler picture in which  $\pi$ -electron delocalization is seen as a prerequisite for strong intramol. coupling. Variations of the coupling with the nature of the bridge (e.g., naphthalene, anthracene, free-base or protonated 1,4,5,8-tetraazaanthracene, tetracene, pyrene, coronene, biphenylene, dicyclobuta[a,d]benzene, dicyclobuta[b,g]naphthalene, dicyclobuta[b,h]biphenylene, and bridges addnl. fused to porphyrin meso positions) and porphyrin (e.g., porphyrin or bacteriochlorin,  $\beta$ -substituents such as methoxy and cyano, Mg, Zn, Ru(CO)<sub>2</sub>, and free-base porphyrins) units are considered, and the phys. origin of quinonoid switching is determined. Terminal alligator clips such as fused phenanthroline, here complexed with CuICl<sub>2</sub>, are also considered.

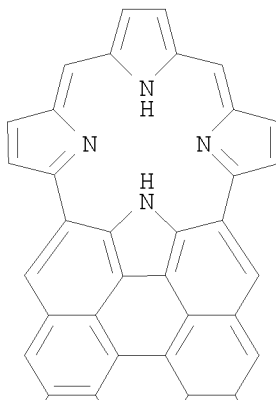
IT 227204-54-8 227204-55-9 227204-56-0  
 227204-67-3 227204-68-4 227204-70-8  
 227204-73-1 227204-74-2 227204-75-3  
 227204-77-5, 33H,35H-Dianthra[2,3-b:2',3'-l]porphine  
 227204-81-1 227204-87-7 227204-88-8  
 227312-50-7 227312-52-9 227312-54-1  
 227312-55-2

RL: PRP (Properties); TEM (Technical or engineered material use); USES (Uses)

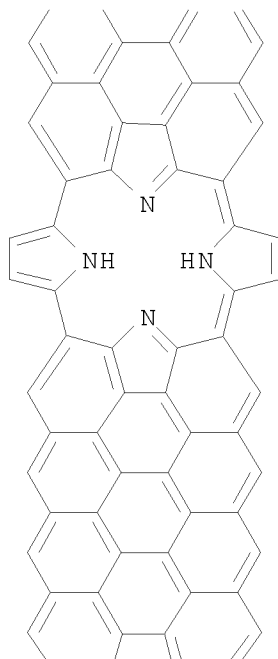
(B3LYP and SCF Calculated Geometric and Electronic Properties of Oligoporphyrin and Related Mols. for mol. wires)

RN 227204-54-8 CAPLUS  
 CN 2,4:19,21:24,26:31,33:36,38:55,53:60,58:65,67-Octametheno-  
 70H,72H,74H,76H,77H,79H-bisporphino[2',3':7,8]coroneno[1,2-b:1',2'-  
 l]porphine (9CI) (CA INDEX NAME)

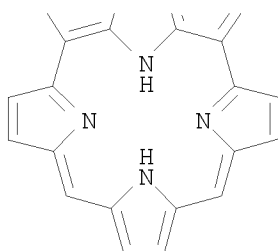
PAGE 1-A



PAGE 2-A

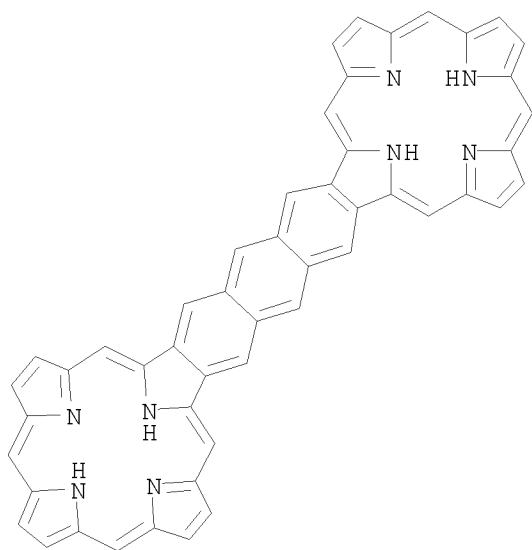


PAGE 3-A

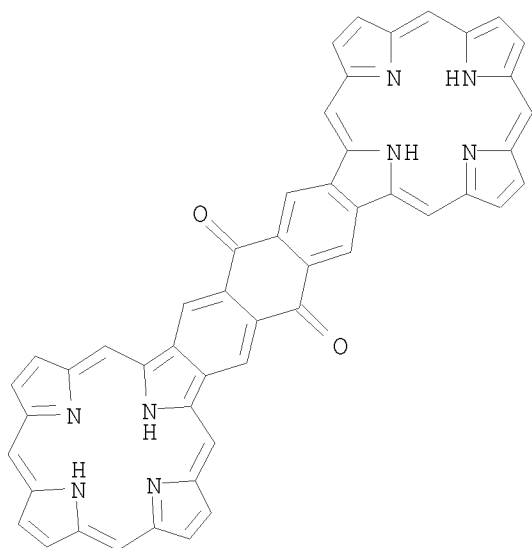


RN 227204-55-9 CAPLUS  
 CN 43H,45H,47H,49H-Anthra[2,3-b:6,7-b']diporphine (9CI) (CA INDEX NAME)

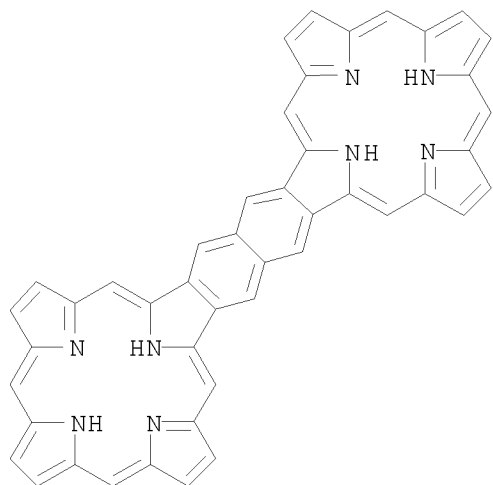




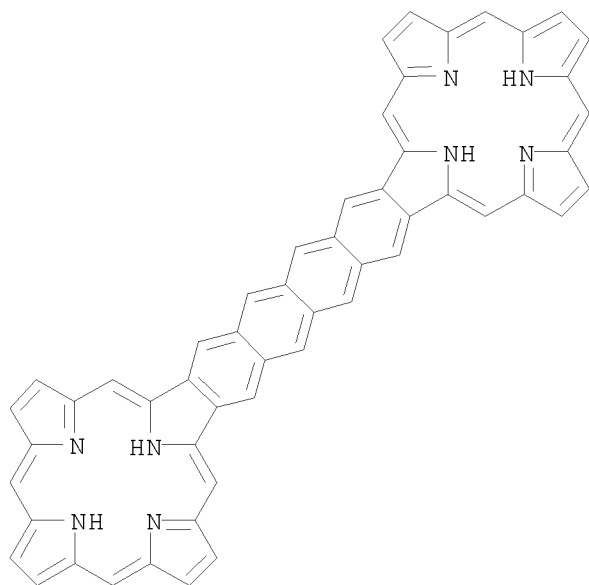
RN 227204-56-0 CAPLUS  
 CN 43H,45H,47H,49H-Anthra[2,3-b:6,7-b']diporphine-20,41-dione (9CI) (CA INDEX NAME)



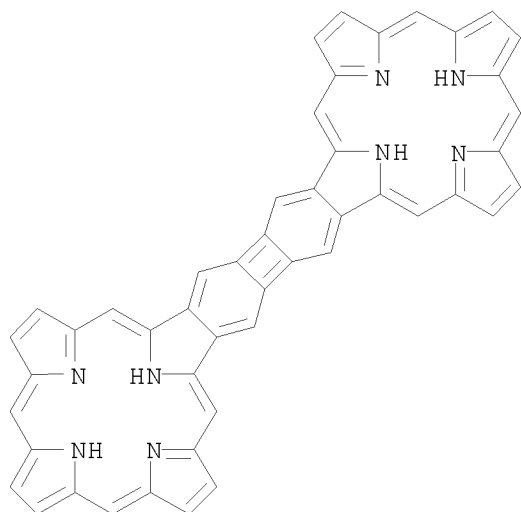
RN 227204-67-3 CAPLUS  
 CN 41H,43H,45H,47H-Naphtho[2,3-b:6,7-b']diporphine (9CI) (CA INDEX NAME)



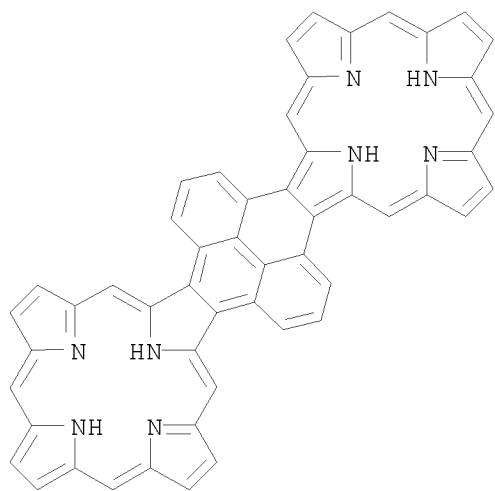
RN 227204-68-4 CAPLUS  
 CN 45H,47H,49H,51H-Naphthaceno[2,3-b:8,9-b']diporphine (9CI) (CA INDEX NAME)



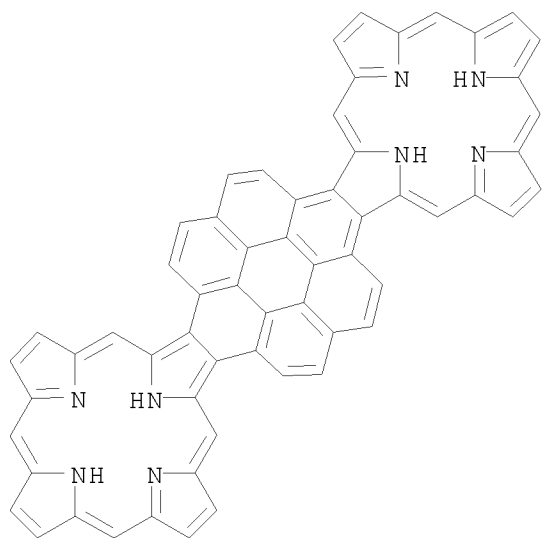
RN 227204-70-8 CAPLUS  
 CN 41H,43H,45H,47H-Biphenyleno[2,3-b:6,7-b']diporphine (9CI) (CA INDEX NAME)



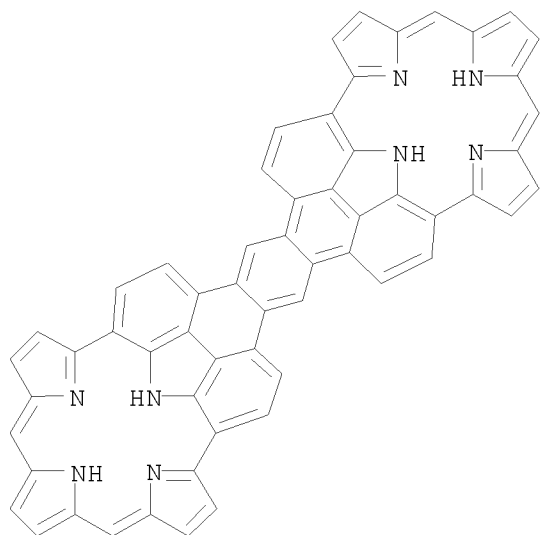
RN 227204-73-1 CAPLUS  
 CN 43H,45H,47H,49H-Pyreno[4,5-b:9,10-b']diporphine (9CI) (CA INDEX NAME)



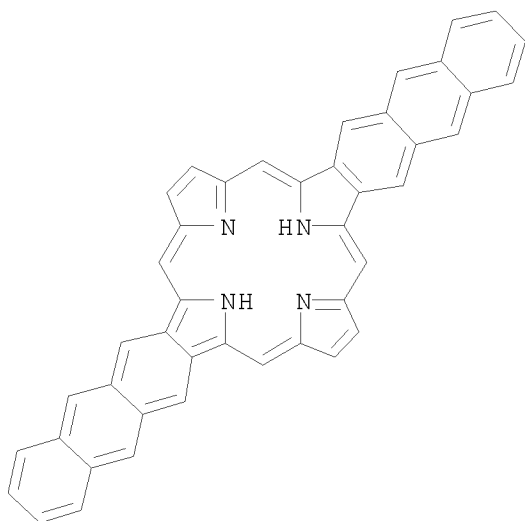
RN 227204-74-2 CAPLUS  
 CN 45H,47H,49H,51H-Coroneno[1,2-b:7,8-b']diporphine (9CI) (CA INDEX NAME)



RN 227204-75-3 CAPLUS  
 CN 2,42:17,19:21,23:38,40-Tetraetheno-43H,45H,47H,49H-anthra[2,3-b:6,7-b']diporphine (9CI) (CA INDEX NAME)

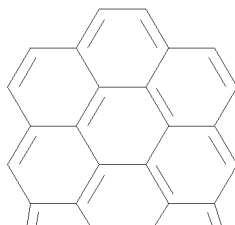


RN 227204-77-5 CAPLUS  
 CN 33H,35H-Dianthra[2,3-b:2',3'-1]porphine (9CI) (CA INDEX NAME)

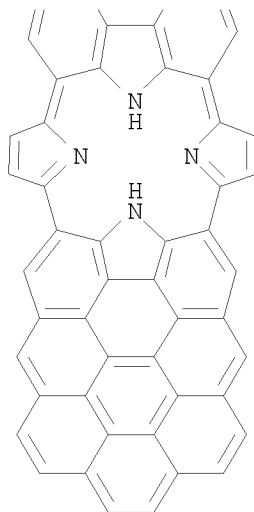


RN 227204-81-1 CAPLUS  
 CN 8,10:15,17:26,28:33,35-Tetrametheno-37H,39H-dicoroneno[1,2-b:1',2'-  
 l]porphine (9CI) (CA INDEX NAME)

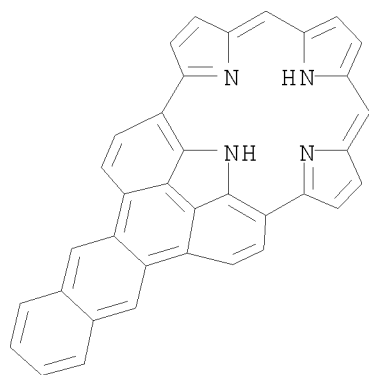
PAGE 1-A



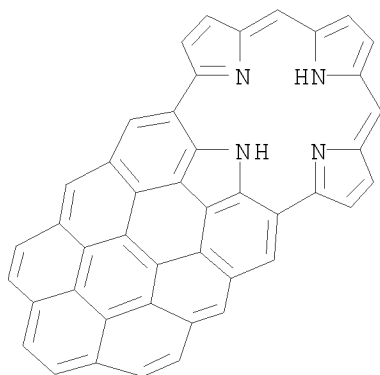
PAGE 2-A



RN 227204-87-7 CAPLUS  
CN 6,8:23,25-Dietheno-27H,29H-anthra[2,3-b]porphine (9CI) (CA INDEX NAME)

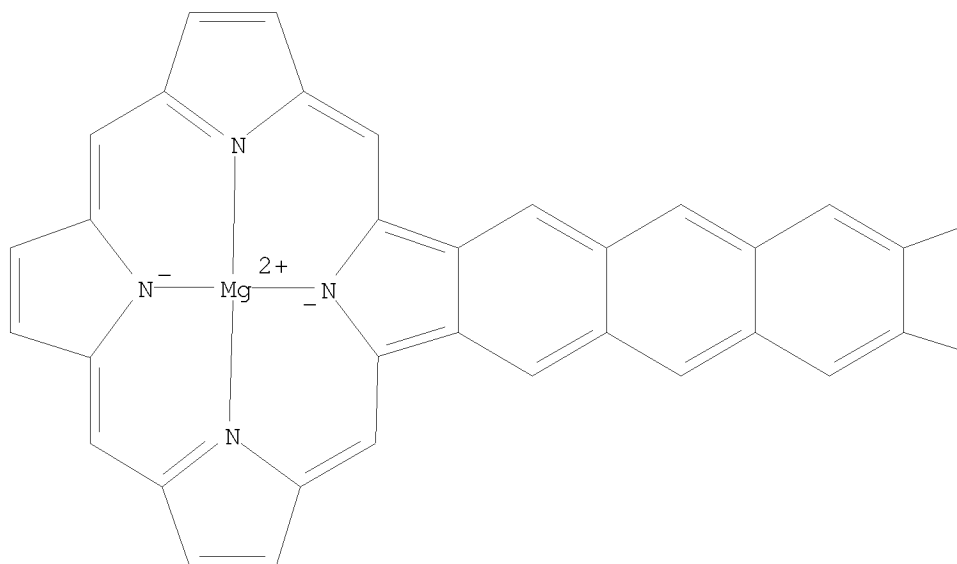


RN 227204-88-8 CAPLUS  
CN 8,10:25,27-Dimetheno-29H,31H-coroneno[1,2-b]porphine (9CI) (CA INDEX NAME)

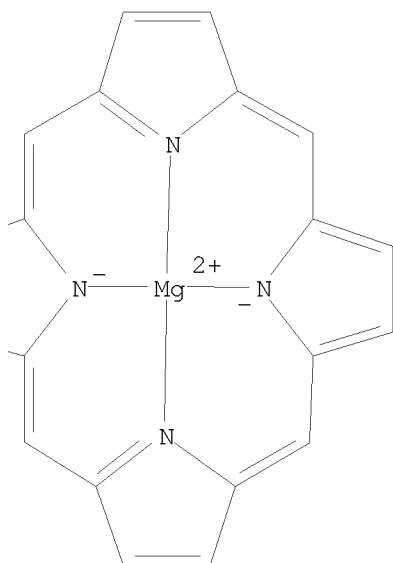


RN 227312-50-7 CAPLUS  
 CN Magnesium, [ $\mu$ -[43H, 45H, 47H, 49H-anthra[2,3-b:6,7-b']diporphinato(4-)-  
 $\kappa$ N43,  $\kappa$ N44,  $\kappa$ N45,  $\kappa$ N46: $\kappa$ N47,  $\kappa$ N48,  $\kappa$ N  
 49,  $\kappa$ N50]]di- (9CI) (CA INDEX NAME)

PAGE 1-A

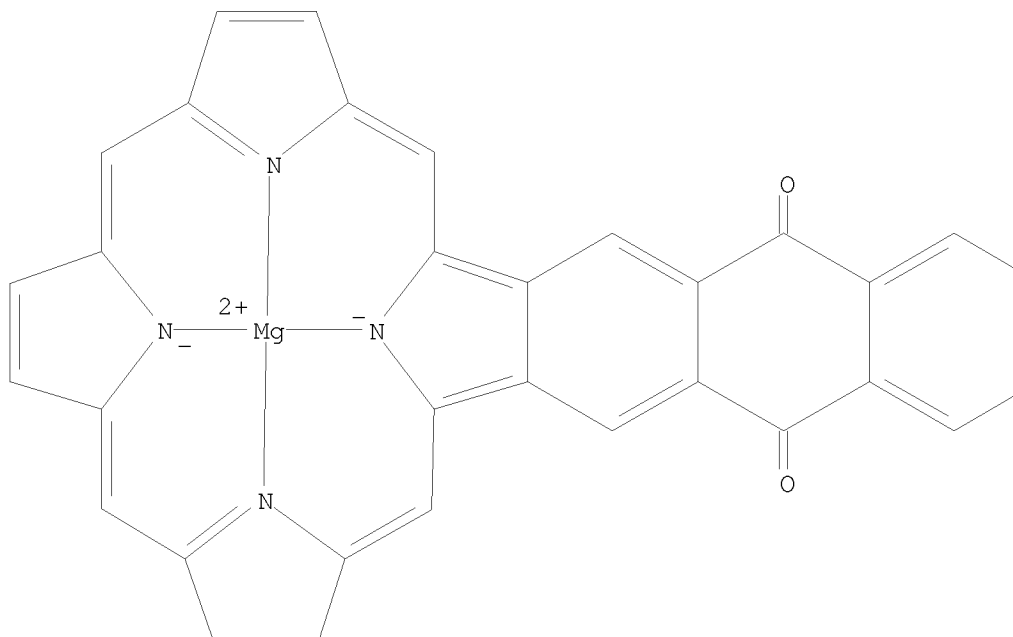


PAGE 1-B



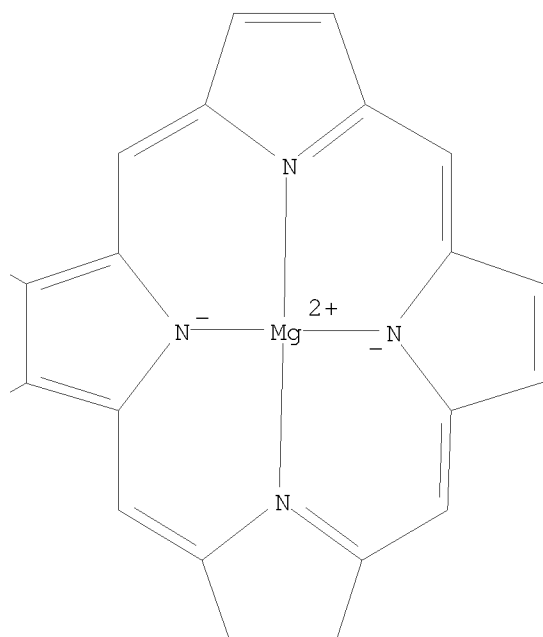
RN 227312-52-9 CAPLUS  
 CN Magnesium, [μ-[43H, 45H, 47H, 49H-anthra[2,3-b:6,7-b']diporphine-20,41-dionato(4-)-κN43,κN44,κN45,κN46:κN47,κN48,κN49,κN50]]di- (9CI) (CA INDEX NAME)

PAGE 1-A





PAGE 1-B



PAGE 2-A

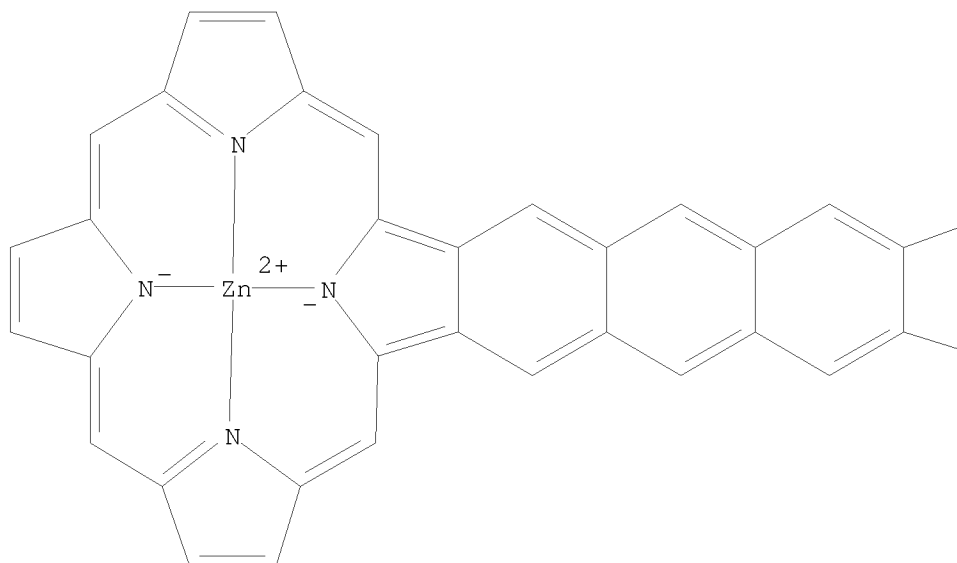


PAGE 2-B

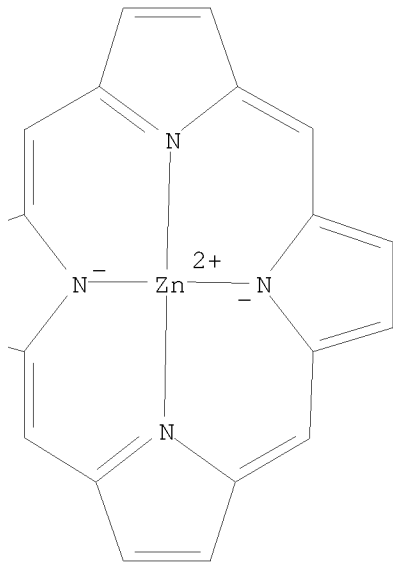


RN 227312-54-1 CAPLUS  
 CN Zinc, [ $\mu$ -[43H,45H,47H,49H-anthra[2,3-b:6,7-b']diporphinato(4-)-  
 $\kappa$ N43, $\kappa$ N44, $\kappa$ N45, $\kappa$ N46: $\kappa$ N47, $\kappa$ N48, $\kappa$ N  
 49, $\kappa$ N50]]di- (9CI) (CA INDEX NAME)

PAGE 1-A

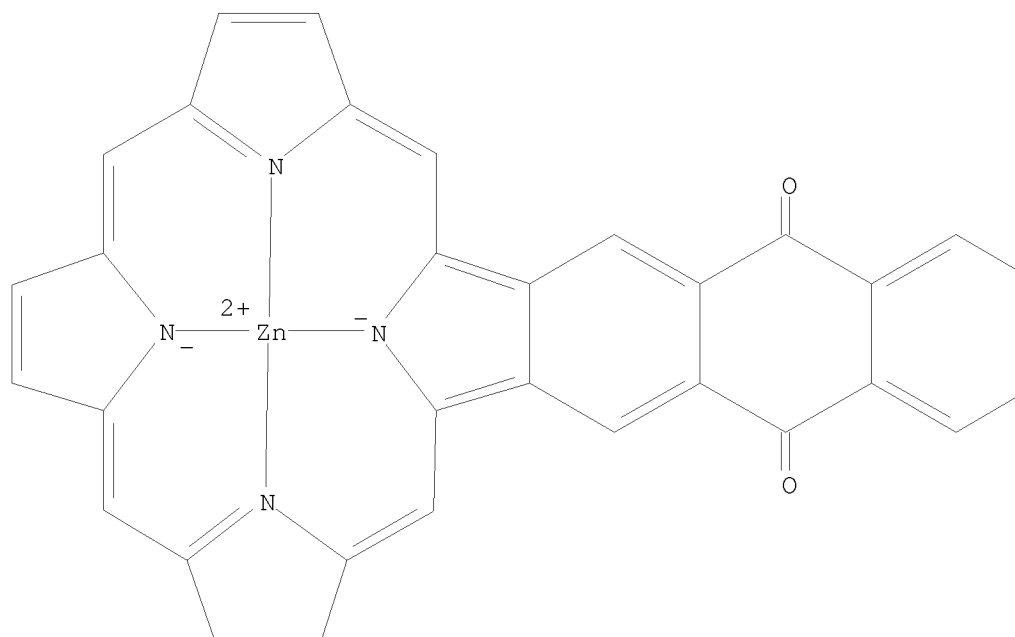


PAGE 1-B

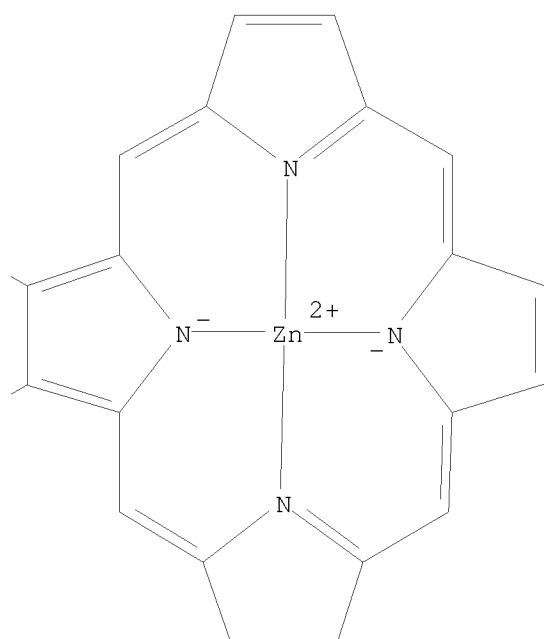


RN 227312-55-2 CAPLUS  
 CN Zinc, [ $\mu$ -[43H, 45H, 47H, 49H-anthra[2,3-b:6,7-b']diporphine-20,41-dionato(4-)- $\kappa$ N43, $\kappa$ N44, $\kappa$ N45, $\kappa$ N46: $\kappa$ N47, $\kappa$ N48, $\kappa$ N49, $\kappa$ N50]]di- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



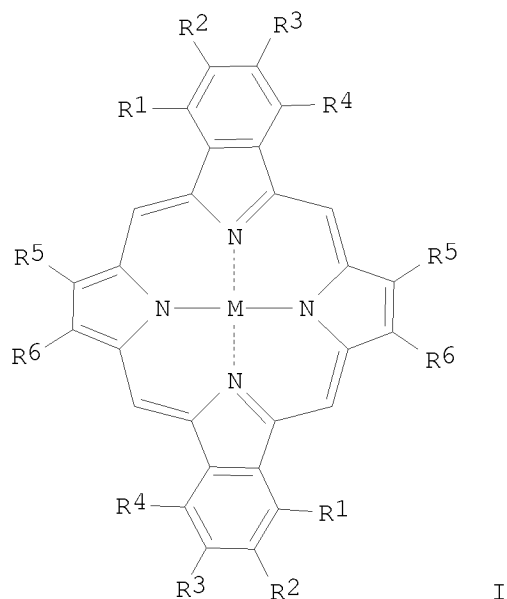
PAGE 2-A

PAGE 2-B

REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 52 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 1999:142144 CAPLUS  
DOCUMENT NUMBER: 130:230045  
TITLE: Optical recording media containing porphyrin compound  
INVENTOR(S): Tsukahara, Hiroshi; Misawa, Tsutami; Sugimoto,  
Kenichi; Nishimoto, Taizo; Tsuda, Takeshi; Umehara,  
Hideki; Takuma, Keisuke  
PATENT ASSIGNEE(S): Mitsui Chemicals Inc., Japan; Yamamoto Chemicals Inc.  
SOURCE: Jpn. Kokai Tokkyo Koho, 11 pp.  
CODEN: JKXXAF  
DOCUMENT TYPE: Patent  
LANGUAGE: Japanese  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
-----	----	-----	-----	-----
JP 11058955	A	19990302	JP 1997-223869	19970820
JP 3704230	B2	20051012		
PRIORITY APPLN. INFO.:			JP 1997-223869	19970820
OTHER SOURCE(S):	MARPAT	130:230045		
GI				



AB The media have a recording layer containing a porphyrin compound I (R1-6 = H, halogen, C1-20 alkyl, alkoxy, alkylthio, aryloxy, arylthio, alkenyl, aralkyl, acyl, aryl; M = two H atoms, divalent metal, tri or tetra valent metal derivative) and a reflection layer on a substrate. The media are useful for recording and rewriting information using laser beam with wavelength 400-500 nm.

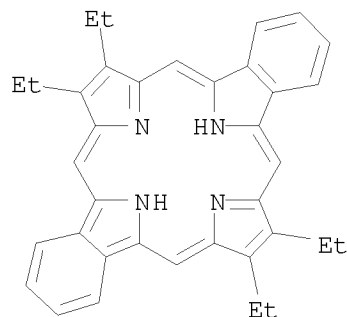
IT 160389-03-7 221109-67-7 221109-68-8  
221109-69-9 221109-70-2 221109-71-3  
221109-72-4 221109-73-5 221109-74-6  
221109-75-7

RL: DEV (Device component use); MOA (Modifier or additive use); USES  
(Uses)

(optical recording media containing porphyrin compound)

RN 160389-03-7 CAPLUS

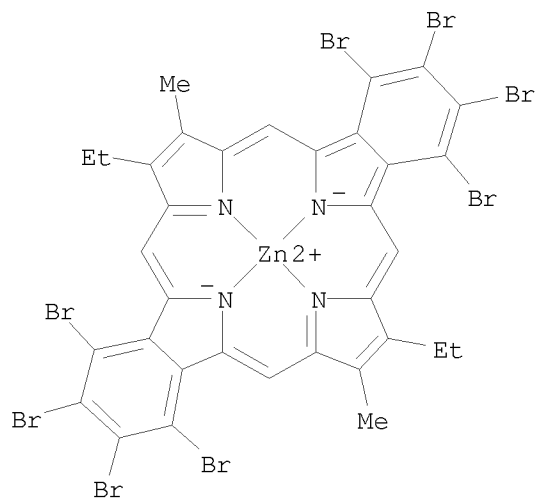
CN 25H,27H-Dibenzo[b,l]porphine, 8,9,20,21-tetraethyl- (9CI) (CA INDEX NAME)



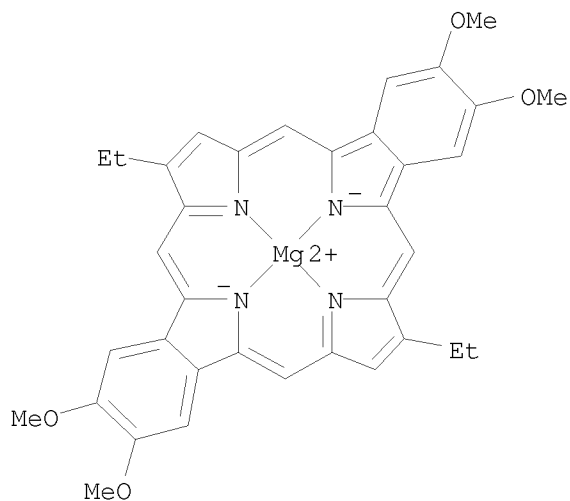
RN 221109-67-7 CAPLUS

CN Zinc, [1,2,3,4,13,14,15,16-octabromo-8,20-diethyl-9,21-dimethyl-25H,27H-

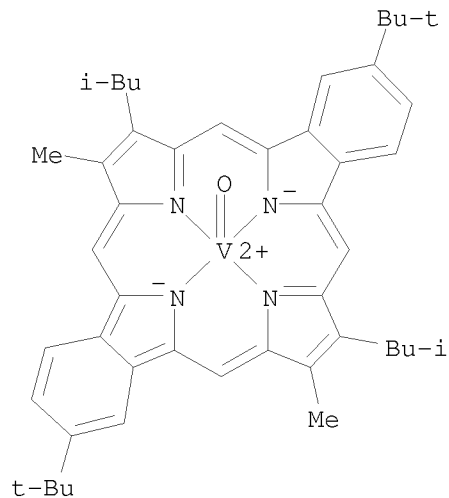
dibenzo[b,1]porphinato(2-)-κN25,κN26,κN27,κN28]-,  
(SP-4-1)-(9CI) (CA INDEX NAME)



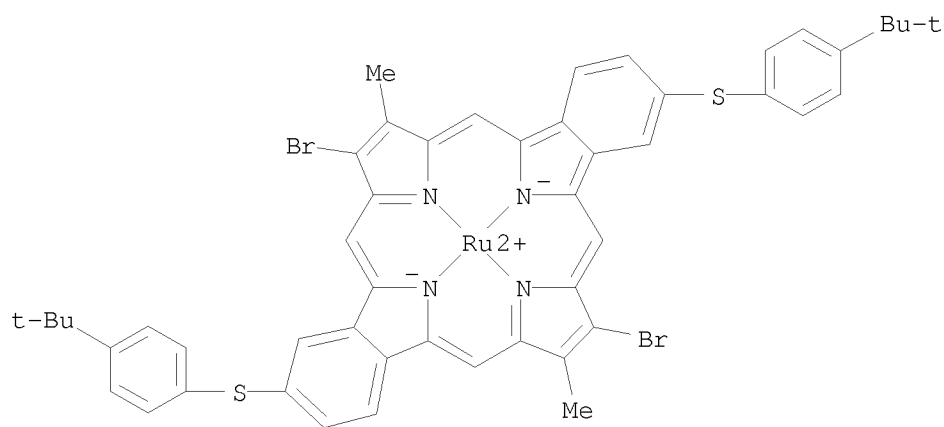
RN 221109-68-8 CAPLUS  
CN Magnesium, [8,20-diethyl-2,3,14,15-tetramethoxy-25H,27H-  
dibenzo[b,1]porphinato(2-)-κN25,κN26,κN27,κN28]-,  
(SP-4-1)-(9CI) (CA INDEX NAME)



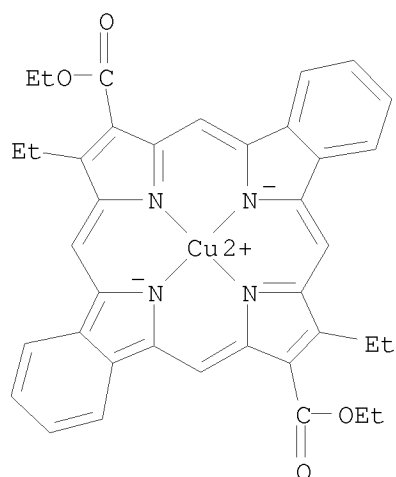
RN 221109-69-9 CAPLUS  
CN Vanadium, [2,14-bis(1,1-dimethylethyl)-9,20-dimethyl-8,21-bis(2-  
methylpropyl)-25H,27H-dibenzo[b,1]porphinato(2-)-  
κN25,κN26,κN27,κN28]oxo-, (SP-5-12)-(9CI) (CA  
INDEX NAME)



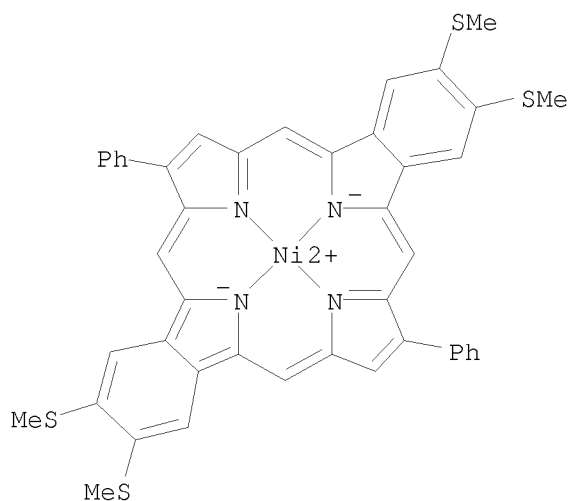
RN 221109-70-2 CAPLUS  
 CN Ruthenium, [9,21-dibromo-2,14-bis[[4-(1,1-dimethylethyl)phenyl]thio]-8,20-dimethyl-25H,27H-dibenzo[b,1]porphinato(2-)-κN25,κN26,κN27,κN28]-, (SP-4-1)-(9CI) (CA INDEX NAME)



RN 221109-71-3 CAPLUS  
 CN Copper, [diethyl 9,21-diethyl-25H,27H-dibenzo[b,1]porphine-8,20-dicarboxylato(2-)-κN25,κN26,κN27,κN28]-, (SP-4-1)-(9CI) (CA INDEX NAME)

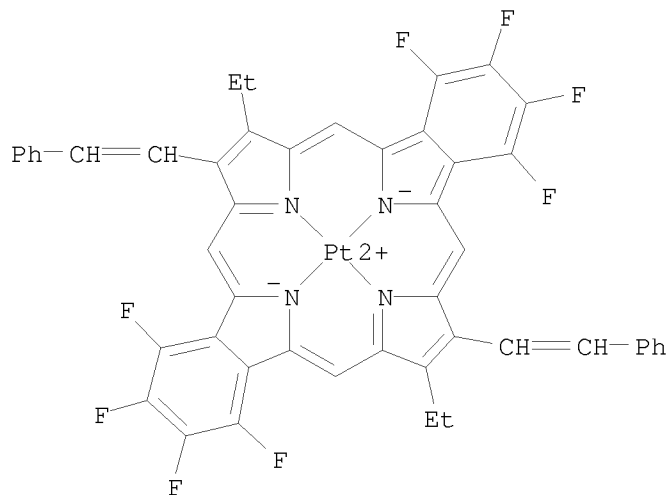


RN 221109-72-4 CAPLUS  
 CN Nickel, [2,3,14,15-tetrakis(methylthio)-8,20-diphenyl-25H,27H-dibenzo[b,1]porphinato(2-)-κN25,κN26,κN27,κN28]-, (SP-4-1)- (9CI) (CA INDEX NAME)

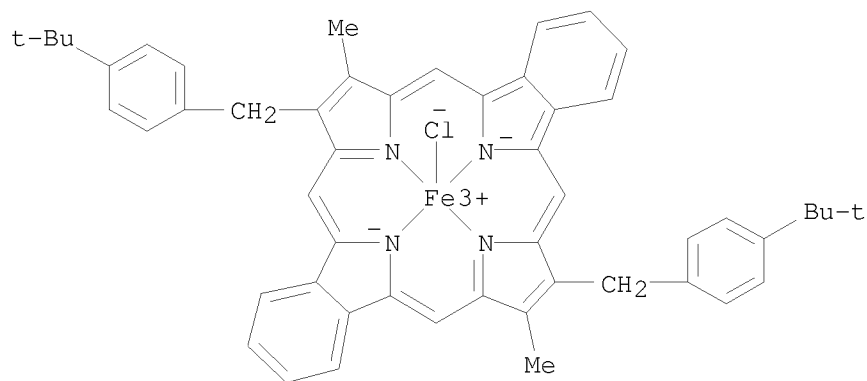


RN 221109-73-5 CAPLUS  
 CN Platinum, [8,20-diethyl-1,2,3,4,13,14,15,16-octafluoro-9,21-bis(2-phenylethenyl)-25H,27H-dibenzo[b,1]porphinato(2-)-κN25,κN26,κN27,κN28]-, (SP-4-1)- (9CI) (CA INDEX NAME)

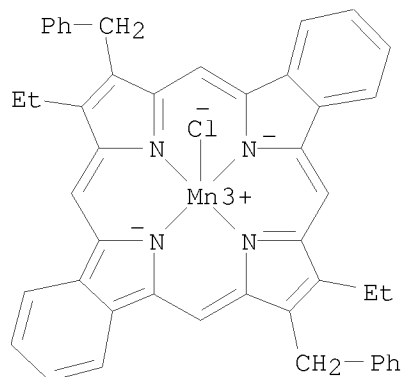




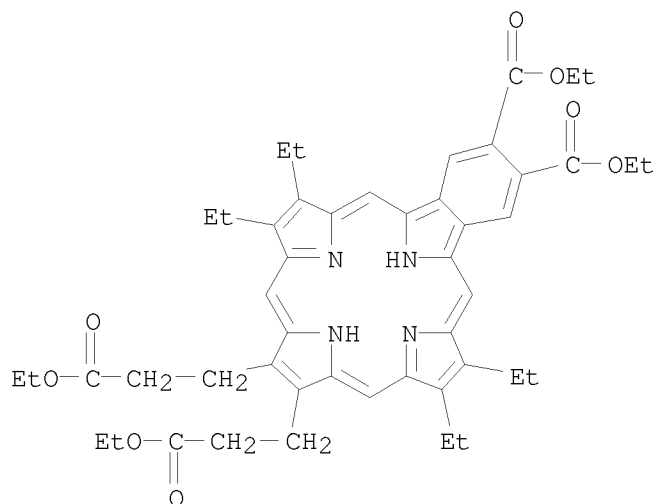
RN 221109-74-6 CAPLUS  
 CN Iron, [8,20-bis[[4-(1,1-dimethylethyl)phenyl]methyl]-9,21-dimethyl-25H,27H-dibenzo[b,1]porphinato(2-)-κN25,κN26,κN27,κN28]chloro-, (SP-5-12)- (9CI) (CA INDEX NAME)



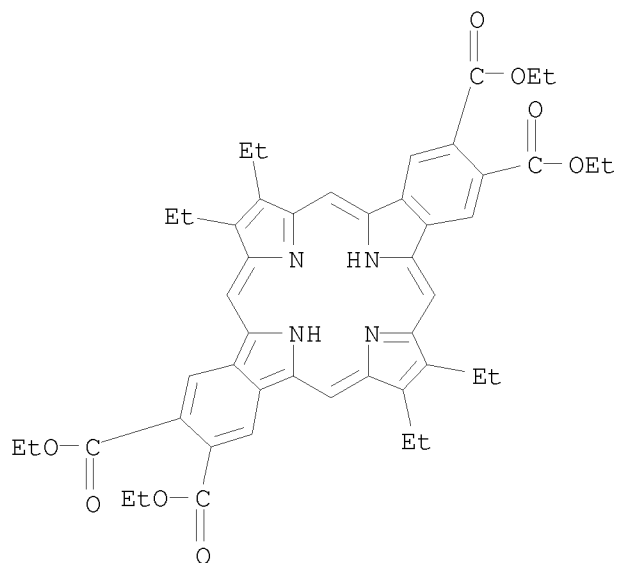
RN 221109-75-7 CAPLUS  
 CN Manganese, chloro[8,20-diethyl-9,21-bis(phenylmethyl)-25H,27H-dibenzo[b,1]porphinato(2-)-κN25,κN26,κN27,κN28]-, (SP-5-12)- (9CI) (CA INDEX NAME)



L9 ANSWER 53 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1998:783175 CAPLUS  
 DOCUMENT NUMBER: 130:124921  
 TITLE: Vic-diacrylic ester porphyrins as starting materials  
 for monobenzoporphyrin and opp-dibenzoporphyrin  
 synthesis  
 AUTHOR(S): Boudif, Arezki; Gimenez, Sandrine; Loock, Bernard;  
 Momenteau, Michel  
 CORPORATE SOURCE: Department of Chemistry, The University of Iowa, Iowa  
 City, IA, 52242-1294, USA  
 SOURCE: Canadian Journal of Chemistry (1998), 76(8), 1215-1219  
 CODEN: CJCHAG; ISSN: 0008-4042  
 PUBLISHER: National Research Council of Canada  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 130:124921  
 AB Synthesis of a bis(vic-diacrylic ester) porphyrin using the "3+1"  
 methodol. is decribed. A two-step procedure is used to convert the  
 vic-diacrylic ester porphyrin and the bis(vic-diacrylic ester) porphyrin  
 to the monobenzoporphyrin and the opp-dibenzoporphyrin, resp.  
 Characterization of the compds. by 1H NMR and UV-visible spectroscopies is  
 also discussed.  
 IT 219858-55-6P 219858-56-7P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (synthesis of monobenzoporphyrin and opp-dibenzoporphyrin starting from  
 vic-diacrylic ester porphyrins)  
 RN 219858-55-6 CAPLUS  
 CN 23H,25H-Benzo[b]porphine-13,14-dipropanoic acid,  
 2,3-bis(ethoxycarbonyl)-8,9,18,19-tetraethyl-, diethyl ester (9CI) (CA  
 INDEX NAME)



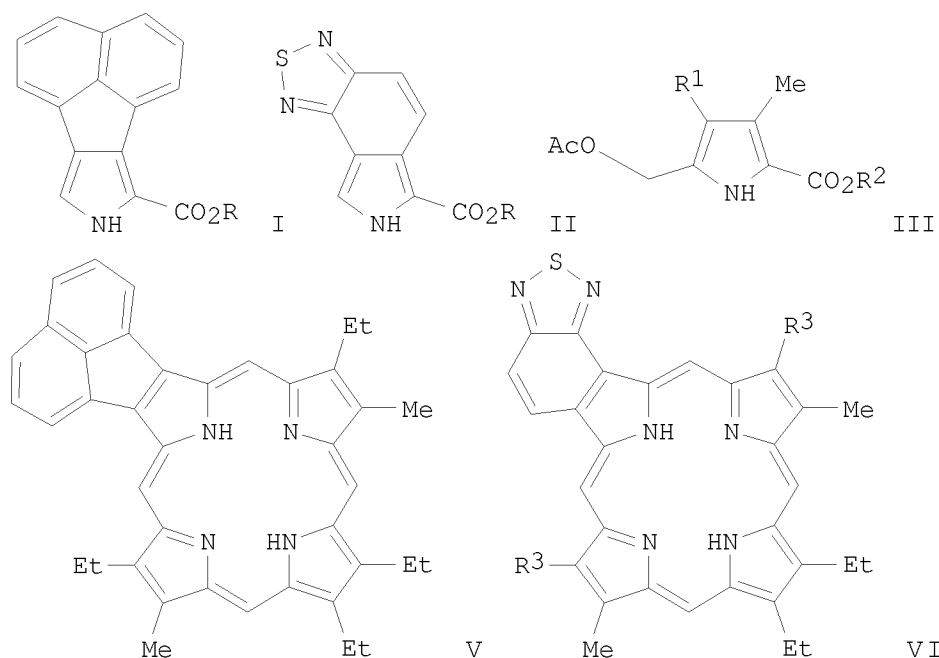
RN 219858-56-7 CAPLUS  
 CN 25H,27H-Dibenzo[b,1]porphine-2,3,14,15-tetracarboxylic acid,  
 8,9,20,21-tetraethyl-, tetraethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 54 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1998:669189 CAPLUS  
 DOCUMENT NUMBER: 130:52257  
 TITLE: Porphyrins with Exocyclic Rings. 13. Synthesis and  
 Spectroscopic Characterization of Highly Modified  
 Porphyrin Chromophores with Fused Acenaphthylene and

AUTHOR(S): Benzothiadiazole Rings  
 Lash, Timothy D.; Chandrasekar, Pushpa; Osuma,  
 Augustine T.; Chaney, Sun T.; Spence, John D.  
 CORPORATE SOURCE: Department of Chemistry, Illinois State University,  
 Normal, IL, 61790-4160, USA  
 SOURCE: Journal of Organic Chemistry (1998), 63(23), 8455-8469  
 CODEN: JOCEAH; ISSN: 0022-3263  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 130:52257  
 GI



AB As part of a survey on the influence of fused aromatic rings on the porphyrin chromophore, a series of novel structures with fused acenaphthylene or benzothiadiazole rings have been synthesized. Base-catalyzed condensation of 1-nitroacenaphthylene or 4-nitrobenzothiadiazole with esters of isocyanoacetic acid afforded good yields of the annelated pyrroles (I) ( $R = Et, CMe_3, CH_2Ph$ ) and (II) ( $R = Et, CMe_3$ ). Cleavage of the ester moieties with KOH in refluxing ethylene glycol gave the unsubstituted heterocycles, and subsequent condensation with 2 equiv of acetoxymethylpyrroles (III) ( $R_1 = Et, CH_2CH_2CO_2Me$ ;  $R_2 = CMe_3, Et, CH_2Ph$ ) in acetic acid/ethanol produced the modified tripyrranes. Tripyrranes with terminal tert-Bu ester units were treated with TFA and condensed with 3,4-diethyl-2,5-pyrroledicarboxaldehyde (IV) in dichloromethane to give, following oxidation with DDQ, the corresponding  $\pi$ -extended porphyrins (V) and (VI) ( $R_3 = Et, CH_2CH_2CO_2Me$ ). Acenaphthoporphyrins V showed unique UV-vis spectra with a triply split Soret band region and a relatively

strong band near 660 nm. Strongly red-shifted absorptions were also noted for the dications and the nickel(II), copper(II), and zinc chelates for this system. Thiadiazoloporphyrins VI gave two broadened Soret bands, but the Q-band region was unexceptional. However, the nickel(II), copper(II), and zinc complexes all showed abnormally strong absorptions between 600 and 612 nm. Porphyrins with two antipodal fused aromatic rings were easily prepared by condensing c-annelated pyrroledialdehydes with tripyrranes and the spectroscopic properties of the resulting porphyrins showed that the observed ring-fusion effects were essentially additive. Porphyrins with two adjacent acenaphthylene rings were also prepared by the MacDonald "2 + 2" condensation, although this chemical gave poor results in the synthesis of a porphyrin with two fused benzothiadiazole rings. The spectroscopic properties of these new highly conjugated porphyrin structures show that ring fusion can profoundly modify the porphyrin chromophore.

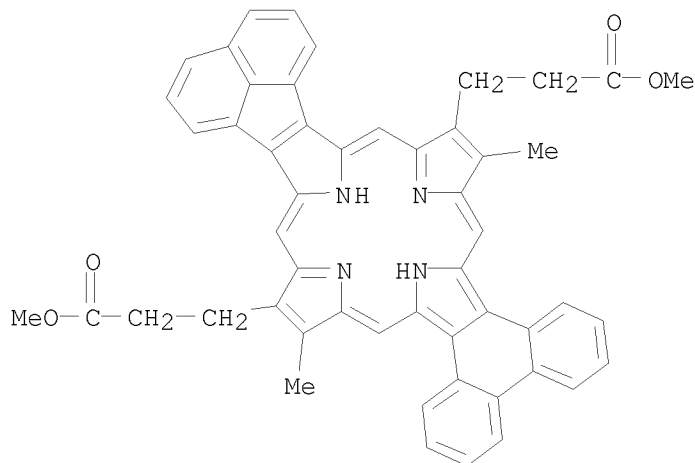
IT 180199-09-1P 217302-11-9P

RL: SPN (Synthetic preparation); PREP (Preparation)

(synthesis and spectroscopic characterization of highly modified porphyrin chromophores with fused acenaphthylene and benzothiadiazole rings)

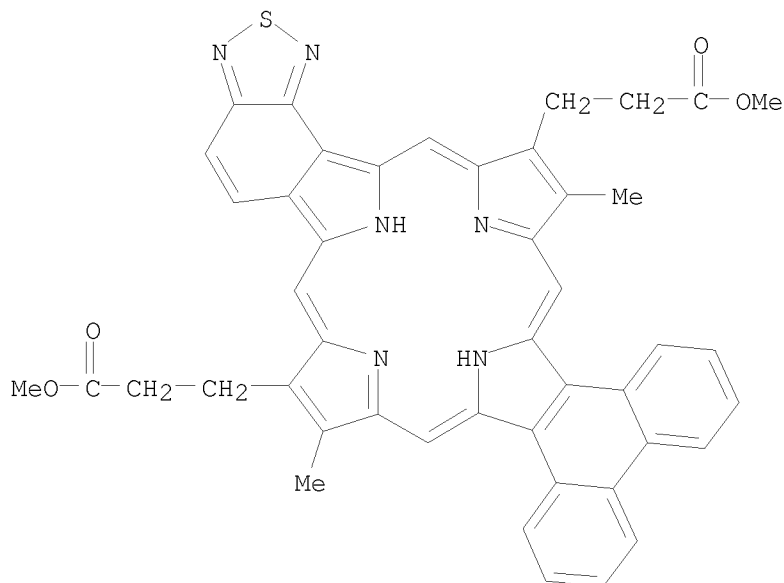
RN 180199-09-1 CAPLUS

CN 31H,33H-Acenaphtho[1,2-b]phenanthro[9,10-1]porphine-13,26-dipropionic acid, 12,27-dimethyl-, dimethyl ester (9CI) (CA INDEX NAME)



RN 217302-11-9 CAPLUS

CN 30H,32H-[2,1,3]Benzothiadiazolo[4,5-b]phenanthro[9,10-1]porphine-13,25-dipropionic acid, 12,26-dimethyl-, dimethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 78 THERE ARE 78 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 55 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1998:504139 CAPLUS

DOCUMENT NUMBER: 129:275753

ORIGINAL REFERENCE NO.: 129:56229a,56232a

TITLE: A new synthesis of benzoporphyrins using 4,7-dihydro-4,7-ethano-2H-isoindole as a synthon of isoindole

AUTHOR(S): Ito, Satoshi; Murashima, Takashi; Ono, Noboru; Uno, Hidemitsu

CORPORATE SOURCE: Faculty of Science, Department of Chemistry, Ehime University, Matsuyama, 790-8577, Japan

SOURCE: Chemical Communications (Cambridge) (1998), (16), 1661-1662

CODEN: CHCOFS; ISSN: 1359-7345

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 129:275753

AB Heating 4,7-dihydro-4,7-ethano-2H-isoindole at 200° induces the retro-Diels-Alder reaction to give isoindole in essentially quant. yield, which can be applied to a new synthesis of tetrabenzoporphyrins and monobenzoporphyrins. Porphyrins and metalloporphyrins were prepared using 4,7-dihydro-4,7-ethano-2H-isoindole which upon heating at 200° for 10 min are converted to benzoporphyrins.

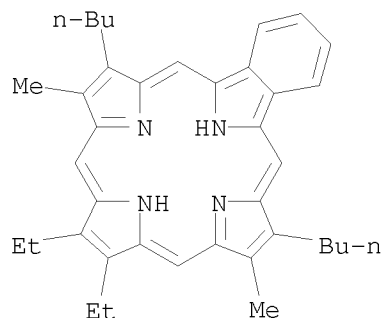
IT 213920-98-0P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of benzoporphyrins by retro-Diels-Alder reaction using ethanoisoindole as synthon of isoindole)

RN 213920-98-0 CAPLUS

CN 23H,25H-Benzo[b]porphine, 8,19-dibutyl-13,14-diethyl-9,18-dimethyl- (9CI)

(CA INDEX NAME)



REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 56 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1998:402309 CAPLUS

DOCUMENT NUMBER: 129:86013

ORIGINAL REFERENCE NO.: 129:17649a,17652a

TITLE: Use of green porphyrins for the manufacture of a medicament for the treatment of secondary cataracts

INVENTOR(S): Meadows, Howard E.; Wenkstern, Danielle; Mallek, David R.; Bussanich, Nick; Richter, Anna M.; Levy, Julia G.; Hariton, Claude A. A.; Huber, Gustav; Rootman, Jack

PATENT ASSIGNEE(S): Qlt Phototherapeutics, Inc., Can.; University of British Columbia; Ciba Vision Corp.

SOURCE: PCT Int. Appl., 49 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9825610	A1	19980618	WO 1997-CA949	19971208
W: AU, CA, CN, CZ, FI, HU, IL, JP, KR, MX, NO, NZ, PL, SK, VN				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
US 6043237	A	20000328	US 1996-762854	19961210
CA 2273010	A1	19980618	CA 1997-2273010	19971208
CA 2273010	C	20070313		
AU 9852202	A	19980703	AU 1998-52202	19971208
AU 737204	B2	20010809		
EP 948329	A1	19991013	EP 1997-946989	19971208
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
CN 1246054	A	20000301	CN 1997-180428	19971208
NZ 336196	A	20001027	NZ 1997-336196	19971208
HU 2000000576	A2	20001128	HU 2000-576	19971208
HU 2000000576	A3	20020930		
JP 2001505885	T	20010508	JP 1998-526039	19971208
ZA 9711104	A	19980710	ZA 1997-11104	19971210
NO 9902808	A	19990809	NO 1999-2808	19990609

MX 9905399	A	20000531	MX 1999-5399	19990610
KR 2000057510	A	20000915	KR 1999-705200	19990610
US 6248734	B1	20010619	US 2000-536291	20000327
PRIORITY APPLN. INFO.:			US 1996-762854	A 19961210
			WO 1997-CA949	W 19971208

OTHER SOURCE(S): MARPAT 129:86013

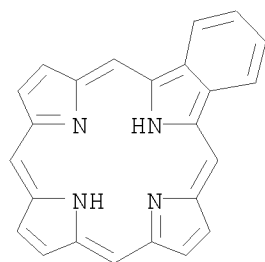
AB In photodynamic therapy to prevent secondary cataracts, green porphyrin photosensitizers are administered to the lens capsule and then irradiated to destroy remnant lens epithelial cells. An amount of green porphyrin sufficient to permit an effective amount to localize in the lens epithelial cells and sufficient time for an effective amount of said green porphyrin to localize in the lens epithelial cells are allowed before irradiating said lens epithelial cells with light absorbed by the green porphyrin at an energy level sufficient to destroy substantially all of the epithelial cells. The green porphyrins offer advantages of rapid uptake by lens epithelial cells, selectivity and effectiveness when employed in protocols directed to the destruction of remnant lens epithelial cells. Thus, human lens epithelial (HLE) cell samples were exposed to 10J/cm<sup>2</sup> red light immediately after a 10 min incubation with a benzoporphyrin derivative (BPD) (a synthetic chlorin-like porphyrin) but subsequent to removal of excess drug. As anticipated, the cell survival was greatly reduced. In in vitro studies, the sensitivity of HLE cells to BPD and light differed depending on donors and number of passages in culture.

IT 36469-17-7D, 23H,25H-Benzo[b]porphine, derivs.

RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
(green porphyrin photosensitizers in photodynamic therapy to prevent secondary cataracts)

RN 36469-17-7 CAPLUS

CN 23H,25H-Benzo[b]porphine (9CI) (CA INDEX NAME)



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 57 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1998:325324 CAPLUS

DOCUMENT NUMBER: 129:54219

ORIGINAL REFERENCE NO.: 129:11301a,11304a

TITLE: Porphyrins with Exocyclic Rings. 11. Synthesis and Characterization of Phenanthroporphyrins, a New Class of Modified Porphyrin Chromophores

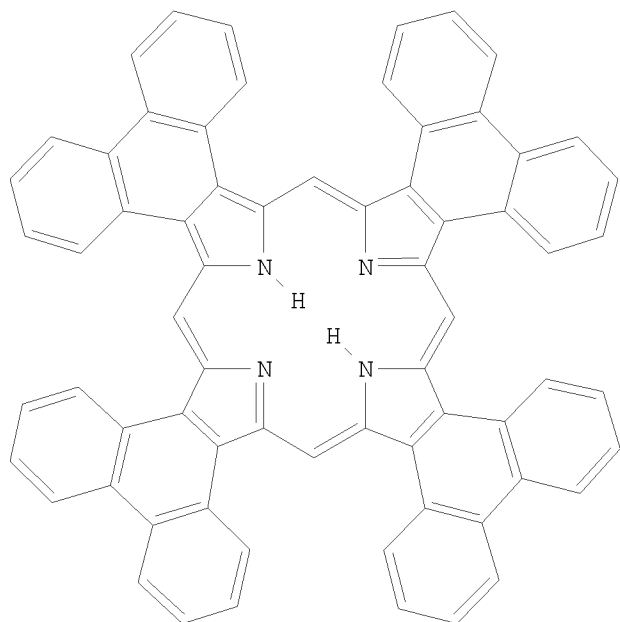
AUTHOR(S): Novak, Bennett H.; Lash, Timothy D.

CORPORATE SOURCE: Department of Chemistry, Illinois State University,  
Normal, IL, 61790-4160, USA

SOURCE: Journal of Organic Chemistry (1998), 63(12), 3998-4010  
CODEN: JOCEAH; ISSN: 0022-3263



PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



I

AB To obtain insights into the factors that influence the electronic spectra of conjugated porphyrin systems, a series of porphyrins with fused phenanthrene subunits have been synthesized. 9-Nitrophenanthrene reacted with esters of isocyanoacetic acid in the presence of DBU in THF to give a series of phenanthro[9,10-c]pyrroles in good to excellent yields, and subsequent acid-catalyzed condensation with various (acetoxymethyl)pyrroles gave six examples of dipyrromethanes that incorporate a fused phenanthrene ring. Cleavage of the benzyl esters by hydrogenolysis over 10% Pd/C gave the corresponding dicarboxylic acid and this condensed with diformyldipyrromethanes under modified MacDonald "2 + 2" condensation conditions to afford the monophenanthroporphyrins. Dipyrromethanes with mixed benzyl and tert-Bu ester moieties were converted into the related formyl dipyrromethanecarboxylic acids, and subsequent head-to-tail self-condensation in the presence of p-toluenesulfonic acid yielded two examples of opp-diphenanthroporphyrins. Reaction of phenanthropyrroles with dimethoxymethane and p-toluenesulfonic acid in acetic acid afforded the sym. dipyrromethanes, and following cleavage of the ester moieties and MacDonald condensation with dialdehyde, the adj-diphenanthroporphyrin was isolated in moderate yield. Metal chelates of the mono-, opp-di-, and adj-diphenanthroporphyrin systems were also prepared, and the electronic spectra for these modified porphyrin systems and their nickel(II), copper(II), and zinc complexes were examined. Surprisingly, the UV-vis absorptions were only slightly shifted to higher wavelengths than those for octaalkylporphyrins. Reduction of Et ester with lithium aluminum hydride gave an unstable carbinol, and subsequent tetramerization in the presence of BF<sub>3</sub> etherate and oxidation with DDQ

afforded the tetraphenanthroporphyrin (I). The free base porphyrin was virtually insol. in organic solvents, but protonation with TFA gave a soluble dication  $I.2H^+$  with a strong Soret band at 482 nm and two weaker absorptions at 615 and 668 nm. The bathochromic shifts for  $I.2H^+$  are far more significant than those observed for the mono- and diphenanthroporphyrin structures, although again somewhat less than might have been expected for this extraordinarily high degree of ring fusion.

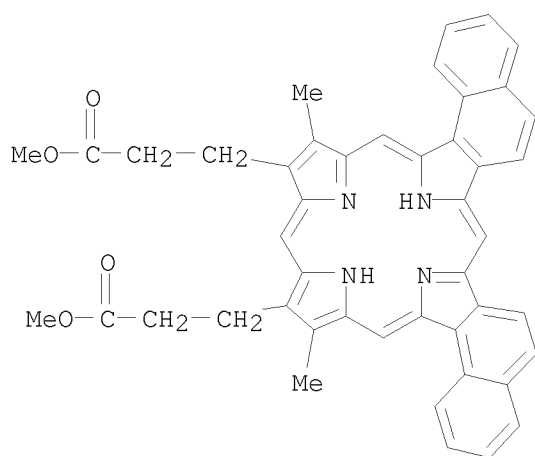
IT 159469-60-0 159469-67-7

RL: PRP (Properties)

(synthesis and characterization of phenanthroporphyrins)

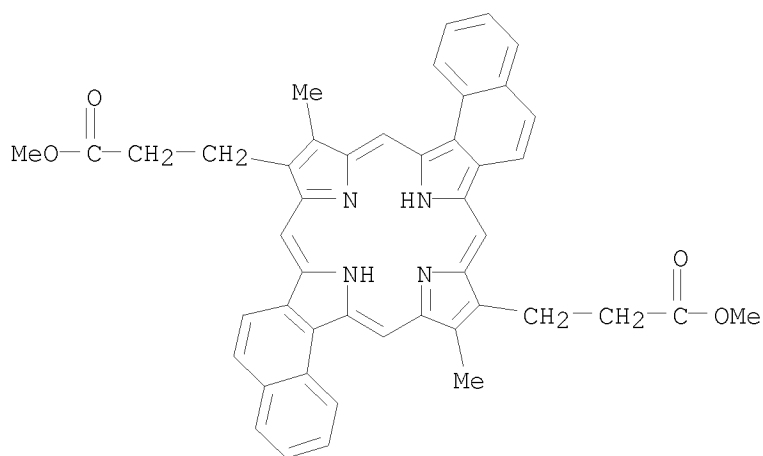
RN 159469-60-0 CAPLUS

CN 29H,31H-Dinaphtho[1,2-b:2',1'-g]porphine-20,24-dipropanoic acid,  
19,25-dimethyl-, dimethyl ester (9CI) (CA INDEX NAME)



RN 159469-67-7 CAPLUS

CN 29H,31H-Dinaphtho[1,2-b:1',2'-l]porphine-10,24-dipropanoic acid,  
11,25-dimethyl-, dimethyl ester (9CI) (CA INDEX NAME)

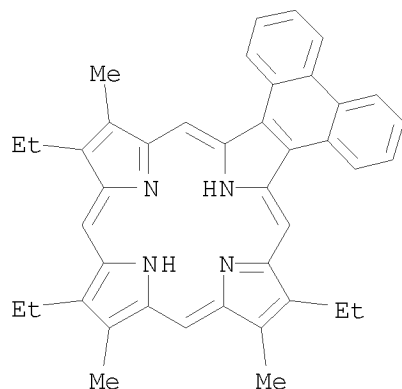


IT 165329-62-4P 165329-66-8P 208578-52-3P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(synthesis and characterization of phenanthroporphyrins)

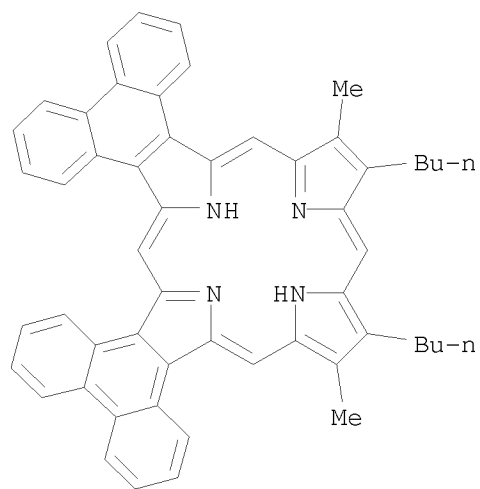
RN 165329-62-4 CAPLUS

CN 27H,29H-Phenanthro[9,10-b]porphine, 12,18,22-triethyl-13,17,23-trimethyl-  
(9CI) (CA INDEX NAME)



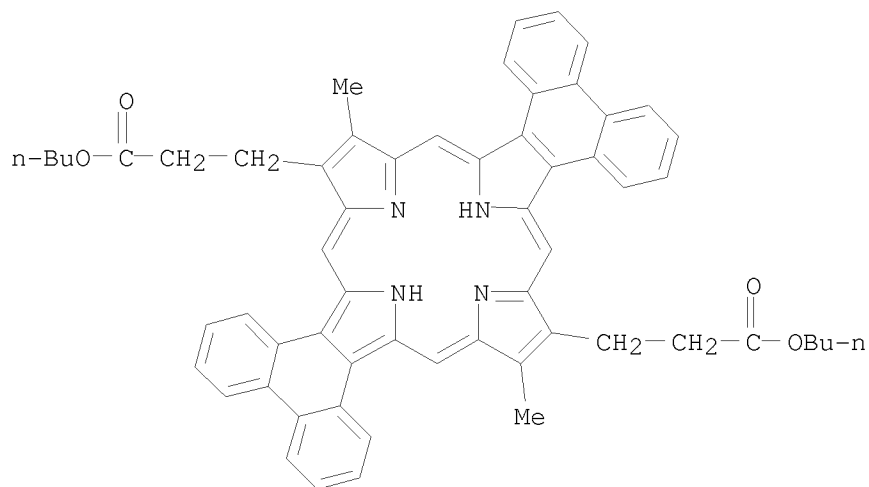
RN 165329-66-8 CAPLUS

CN 33H,35H-Diphenanthro[9,10-b:9',10'-g]porphine, 9,13-dibutyl-8,14-dimethyl-  
(9CI) (CA INDEX NAME)

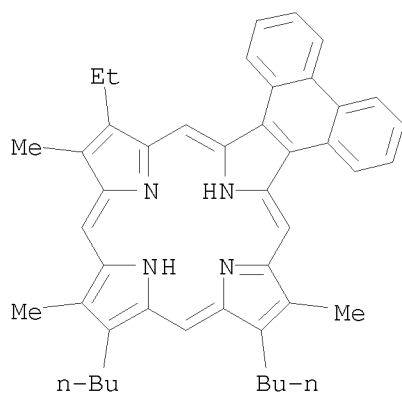


RN 208578-52-3 CAPLUS

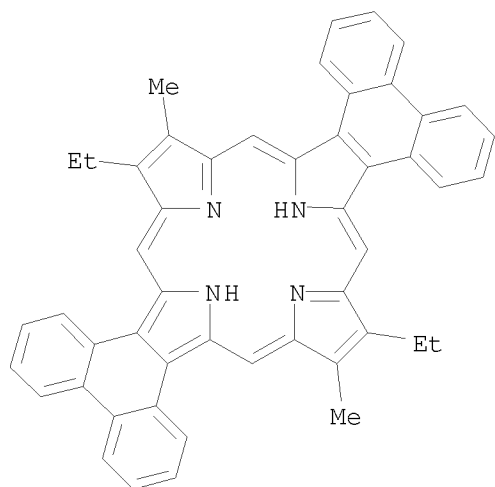
CN 33H,35H-Diphenanthro[9,10-b:9',10'-l]porphine-12,28-dipropionic acid,  
13,29-dimethyl-, dibutyl ester (9CI) (CA INDEX NAME)



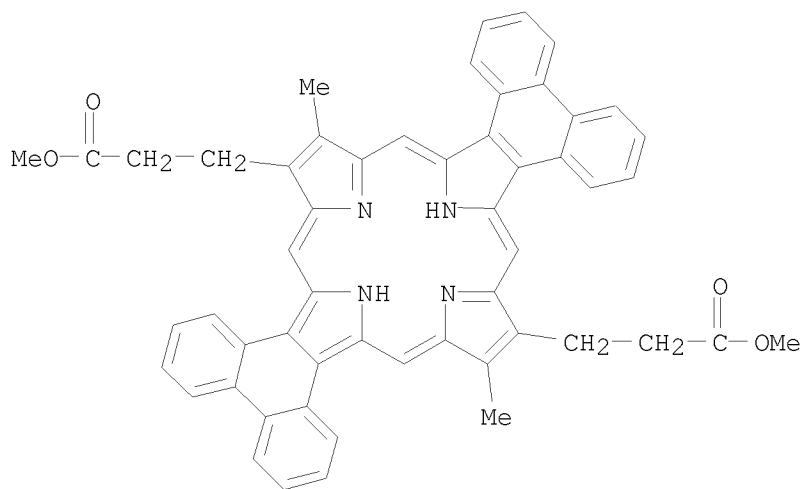
IT 165329-63-5P 165329-64-6P 165329-65-7P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (synthesis and characterization of phenanthroporphyrins)  
 RN 165329-63-5 CAPLUS  
 CN 27H,29H-Phenanthro[9,10-b]porphine,  
 13,17-dibutyl-23-ethyl-12,18,22-trimethyl- (9CI) (CA INDEX NAME)



RN 165329-64-6 CAPLUS  
 CN 33H,35H-Diphenanthro[9,10-b:9',10'-l]porphine,  
 12,28-diethyl-13,29-dimethyl- (9CI) (CA INDEX NAME)



RN 165329-65-7 CAPLUS  
 CN 33H,35H-Diphenanthro[9,10-b:9',10'-1]porphine-12,28-dipropionic acid,  
 13,29-dimethyl-, dimethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 99 THERE ARE 99 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 58 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1997:733390 CAPLUS  
 DOCUMENT NUMBER: 128:42910  
 ORIGINAL REFERENCE NO.: 128:8255a,8258a  
 TITLE: Elemental sulfur-porphyrin interactions  
 AUTHOR(S): Rohrer, Annick; Ocampo, Ruben; Callot, Henry J.  
 CORPORATE SOURCE: Faculte de Chimie, URA 31 associee au CNRS, Universite  
 Louis Pasteur, Strasbourg, 67008, Fr.  
 SOURCE: Bulletin de la Societe Chimique de France (1997),  
 134(7), 689-696

CODEN: BSCFAS; ISSN: 0037-8968

PUBLISHER: Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

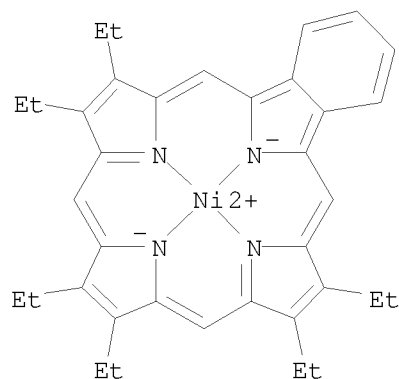
AB To mimic geochem. processes, several alkylporphyrins were heated in the presence of elemental S >200°. A variety of products were observed, and thiopyrano- and thienylporphyrins as well as dealkylated, homologated and dehydrogenated porphyrins were characterized.

IT 199176-05-1P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 199176-05-1 CAPLUS

CN Nickel, [8,9,13,14,18,19-hexaethyl-23H,25H-benzo[b]porphinato(2-)-  
κN23,κN24,κN25,κN26]-, (SP-4-1)- (9CI) (CA INDEX  
NAME)



REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 59 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1997:470280 CAPLUS

DOCUMENT NUMBER: 127:149026

ORIGINAL REFERENCE NO.: 127:28789a,28792a

TITLE: meso-Arylporphyrins as dienophiles in Diels-Alder reactions: a novel approach to the synthesis of

chlorins, bacteriochlorins and naphthoporphyrins

AUTHOR(S): Tome, Augusto C.; Lacerda, Paula S. S.; Neves, Maria G. P. M. S.; Cavaleiro, Jose A. S.

CORPORATE SOURCE: Dep. Chem., Univ. Aveiro, Aveiro, 3810, Port.

SOURCE: Chemical Communications (Cambridge) (1997), (13),  
1199-1200

CODEN: CHCOFS; ISSN: 1359-7345

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Meso-Arylporphyrins participate, as dienophiles, in Diels-Alder reactions with o-benzoquinodimethane to yield novel chlorins, bacteriochlorins and naphtho[2,3-b]porphyrins.

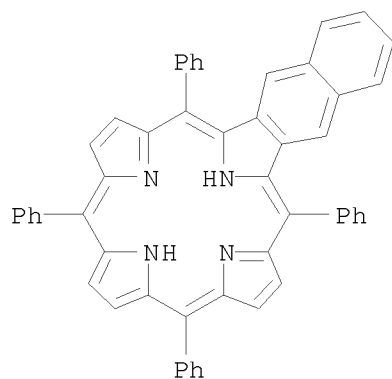
IT 193283-52-2P 193283-66-8P 193283-69-1P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(synthesis of chlorins, bacteriochlorins and naphthoporphyrins through

Diels-Alder reactions of meso-arylporphyrins with  
o-benzoquinodimethane)

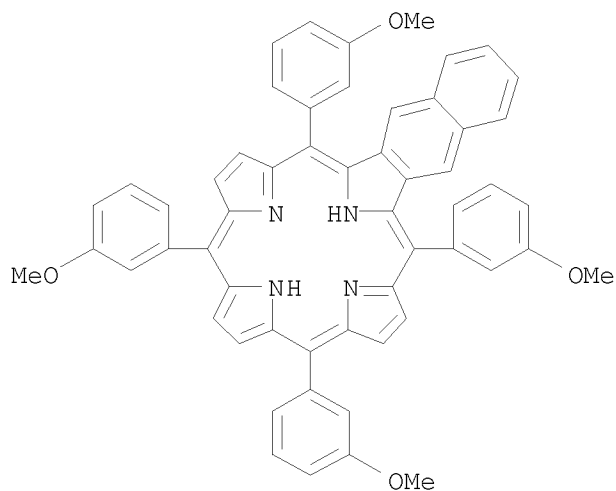
RN 193283-52-2 CAPLUS

CN 25H,27H-Naphtho[2,3-b]porphine, 7,12,17,22-tetraphenyl- (CA INDEX NAME)



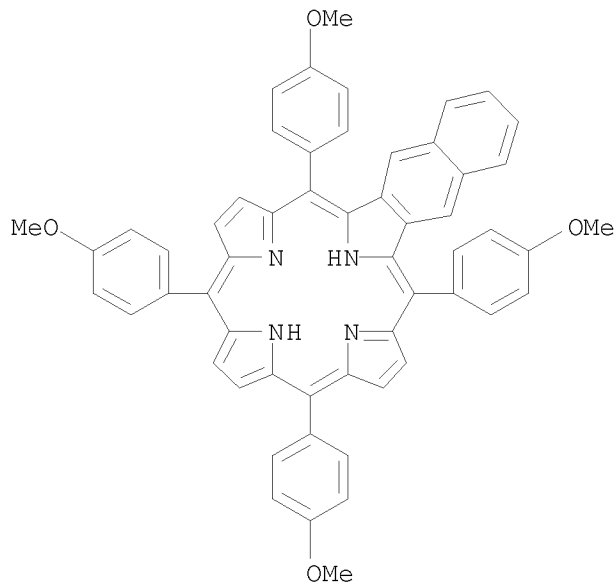
RN 193283-66-8 CAPLUS

CN 25H,27H-Naphtho[2,3-b]porphine, 7,12,17,22-tetrakis(3-methoxyphenyl)-  
(9CI) (CA INDEX NAME)



RN 193283-69-1 CAPLUS

CN 25H,27H-Naphtho[2,3-b]porphine, 7,12,17,22-tetrakis(4-methoxyphenyl)-  
(9CI) (CA INDEX NAME)



REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 60 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1997:215938 CAPLUS

DOCUMENT NUMBER: 126:293213

ORIGINAL REFERENCE NO.: 126:56781a, 56784a

TITLE: Synthesis of novel porphyrin chromophores from nitroarenes: further applications of the Barton-Zard pyrrole condensation

AUTHOR(S): Lash, Timothy D.; Wijesinghe, Chaminda; Osuma, Augustine T.; Patel, Jyoti R.

CORPORATE SOURCE: Dep. Chemistry, Illinois State Univ., Normal, IL, 61790-4160, USA

SOURCE: Tetrahedron Letters (1997), 38(12), 2031-2034  
CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 126:293213

GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB Porphyrins with fused nitronaphthalene I and benzothiadiazole subunits II (R = Et, Bu), were synthesized by the "2 + 2" and "3 + 1" methodologies; the key pyrrolic intermediates were prepared by the base catalyzed condensation of dinitronaphthalenes or 4-nitro-2,1,3-benzothiadiazole with isocyanoacetates.

IT 189124-64-9P

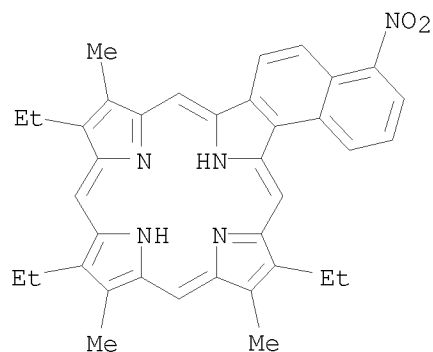
RL: SPN (Synthetic preparation); PREP (Preparation)



(synthesis of novel porphyrin chromophores from nitroarenes via  
Barton-Zard pyrrole condensation)

RN 189124-64-9 CAPLUS

CN 25H,27H-Naphtho[1,2-b]porphine, 11,15,21-triethyl-10,16,20-trimethyl-4-nitro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 61 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1996:668617 CAPLUS

DOCUMENT NUMBER: 126:47008

ORIGINAL REFERENCE NO.: 126:9265a,9268a

TITLE: Approaches to the stepwise synthesis of  
benzoporphyrins and phthalocyanines. Part 1. Synthesis  
of opp-dibenzoporphyrins (dibenzo[g,q]porphyrins)

AUTHOR(S): Bonnett, Raymond; McManus, Kimberly A.

CORPORATE SOURCE: Chem. Dep., Queen Mary and Westfield College, London,  
E1 4NS, UK

SOURCE: Journal of the Chemical Society, Perkin Transactions  
1: Organic and Bio-Organic Chemistry (1996), (20),  
2461-2466

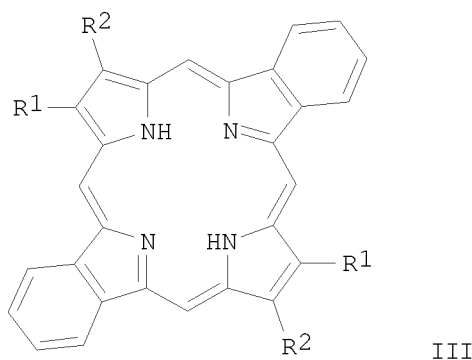
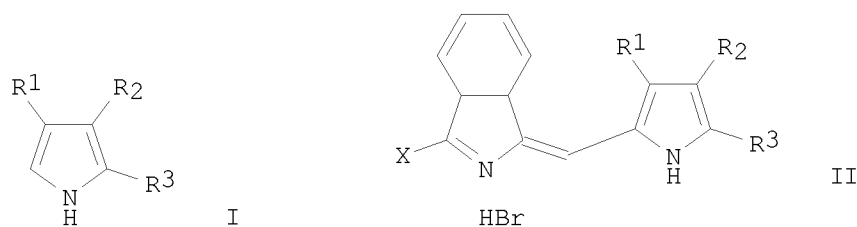
CODEN: JCPRB4; ISSN: 0300-922X

PUBLISHER: Royal Society of Chemistry

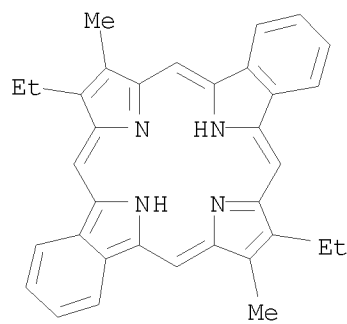
DOCUMENT TYPE: Journal

LANGUAGE: English

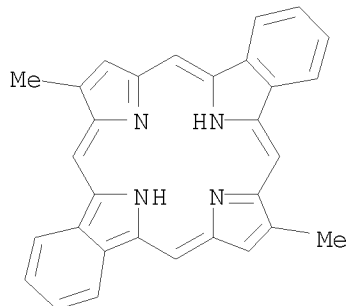
GI



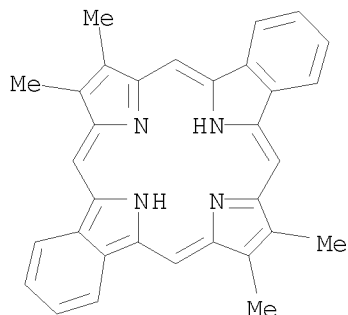
- AB A stepwise synthesis of the opp-dibenzoporphyrin (dibenzo[g,q]porphyrin) system involving isoindole precursors is described. 3-Halogeno-1-formylisoindoles are condensed with various  $\alpha$ -unsubstituted pyrroles I ( $R_1$  = Me, Et;  $R_2$  = H, Me, Et, CO<sub>2</sub>Et;  $R_3$  = H, Me) to give the corresponding benzopyrromethene hydrobromides II ( $X$  = Cl, Br). Thermal self-condensation of such compds. bearing an  $\alpha$ -Me group gives the corresponding opp-dibenzoporphyrin derivs. (III) in low to modest yields depending on the  $\beta$ -substitution pattern of the original pyrrole component.
- IT 81976-22-9P 157869-31-3P 157869-32-4P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(synthesis of opp-dibenzoporphyrins (dibenzo[g,q]porphyrins))
- RN 81976-22-9 CAPLUS
- CN 25H,27H-Dibenzo[b,l]porphine, 8,20-diethyl-9,21-dimethyl- (9CI) (CA INDEX NAME)



RN 157869-31-3 CAPLUS  
CN 25H,27H-Dibenzo[b,l]porphine, 8,20-dimethyl- (9CI) (CA INDEX NAME)



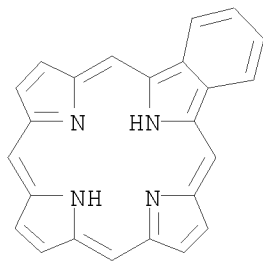
RN 157869-32-4 CAPLUS  
CN 25H,27H-Dibenzo[b,l]porphine, 8,9,20,21-tetramethyl- (9CI) (CA INDEX NAME)



L9 ANSWER 62 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 1996:567252 CAPLUS  
DOCUMENT NUMBER: 125:219600  
ORIGINAL REFERENCE NO.: 125:41075a  
TITLE: Green porphyrins as immunomodulators  
INVENTOR(S): Chan, Anges How-Ching; Hunt, David William Carey;  
Levy, Julia; Obochi, Modestus Onuora Kay; Richter,  
Anna; Simkin, Guillermo O.  
PATENT ASSIGNEE(S): Quadra Logic Technologies Inc., Can.  
SOURCE: PCT Int. Appl., 32 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 5  
PATENT INFORMATION:

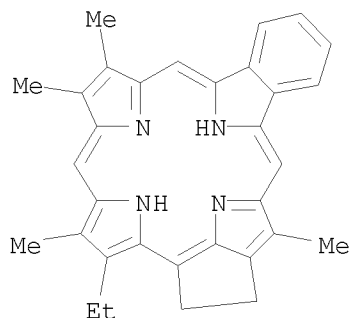
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9622090	A1	19960725	WO 1996-CA20	19960111
W: AU, CA, CN, CZ, FI, HU, JP, KR, MX, NO, NZ, PL, SK				

RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE  
 US 5789433 A 19980804 US 1995-374158 19950117  
 TW 384222 B 20000311 TW 1995-84113793 19951221  
 CA 2210152 A1 19960725 CA 1996-2210152 19960111  
 CA 2210152 C 20070403  
 AU 9643819 A 19960807 AU 1996-43819 19960111  
 AU 706796 B2 19990624  
 EP 794775 A1 19970917 EP 1996-900221 19960111  
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE  
 HU 9801528 A2 19981028 HU 1998-1528 19960111  
 HU 9801528 A3 20000228  
 CN 1198671 A 19981111 CN 1996-191441 19960111  
 JP 10512268 T 19981124 JP 1996-521931 19960111  
 JP 3574456 B2 20041006  
 NZ 298356 A 20010427 NZ 1996-298356 19960111  
 CZ 291179 B6 20030115 CZ 1997-2213 19960111  
 FI 9702952 A 19970910 FI 1997-2952 19970711  
 NO 9703293 A 19970916 NO 1997-3293 19970716  
 PRIORITY APPLN. INFO.: US 1995-374158 A 19950117  
 WO 1996-CA20 W 19960111  
 OTHER SOURCE(S): MARPAT 125:219600  
 AB Green porphyrins act as antigen-specific immunomodulators in the active  
 phase of an immune response to a particular antigen, as well as to  
 interfere with intracellular communication. These effects occur in the  
 absence of radiation absorbed by the green porphyrin. In example, the  
 effect of BPD, BPD-MB or BPD-MA (benzoporphyrin derivative in monoacid or  
 monobase form) on exptl. allergic encephalomyelitis, on delayed-type  
 hypersensitivity, on fibrinogen binding, on skin allograft rejection, on  
 ICAM-1 in rheumatoid arthritis, and on integrin binding was tested.  
 IT 36469-17-7D, 23H,25H-Benzo[b]porphine, derivs.  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological  
 study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES  
 (Uses)  
 (green porphyrins as immunomodulators for antigen-specific immune  
 responses)  
 RN 36469-17-7 CAPLUS  
 CN 23H,25H-Benzo[b]porphine (9CI) (CA INDEX NAME)



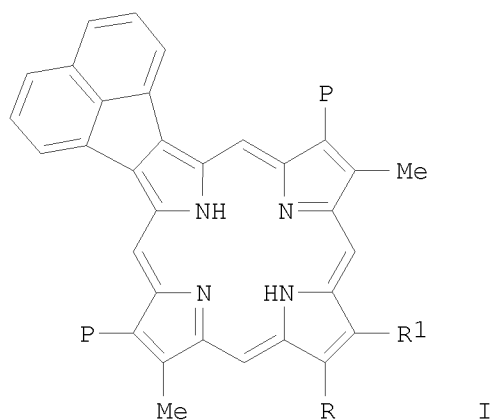
L9 ANSWER 63 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1996:522915 CAPLUS  
 DOCUMENT NUMBER: 125:304707  
 ORIGINAL REFERENCE NO.: 125:56945a,56948a  
 TITLE: High-performance liquid chromatography-mass  
 spectrometry of porphyrins by using an atmospheric

pressure interface  
 AUTHOR(S): Rosell-Mele, Antoni; Carter, James F.; Maxwell, James R.  
 CORPORATE SOURCE: Organic Geochemistry Unit, Univ. Bristol, Bristol, BS8 1TS, UK  
 SOURCE: Journal of the American Society for Mass Spectrometry (1996), 7(9), 965-971  
 CODEN: JAMSEF; ISSN: 1044-0305  
 PUBLISHER: Elsevier  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB A method was described for the high-performance liquid chromatog. (HPLC)-mass spectrometry anal. of porphyrin mixts. using an atmospheric pressure interface, which can operate in two modes: pneumatically assisted electrospray and atmospheric pressure chemical ionization (APCI).  
 Optimization of the conditions and evaluation of spectral information was carried out using direct injection of free-base and metallo porphyrin stds. The most effective results were obtained with APCI. HPLC-APCI mass spectrometry anal. of the demetalated vanadyl porphyrin fraction from Triassic Serpiano oil shale has allowed rapid characterization of the distribution; >50 significant components were present. The presence of trace amts. of high-mol.-weight (C>33) cycloalkano porphyrins indicated the occurrence of photic zone anoxia in the ancient water column. This example illustrated the potential of this approach for studies of porphyrin mixts. of environmental or biol. significance, which should be applicable to other types of metallo and free-base components that can be separated by HPLC under normal or reversed-phase conditions.  
 IT 100813-32-9  
 RL: ANT (Analyte); GOC (Geological or astronomical occurrence); ANST (Analytical study); OCCU (Occurrence)  
 (high-performance liquid chromatog.-chemical ionization mass spectroscopy of porphyrins in oil shale)  
 RN 100813-32-9 CAPLUS  
 CN 5,22:12,15-Diimino-20,18-metheno-7,10-nitrilobenzo[o]cyclopent[b]azacyclononadecine, 14-ethyl-16,17-dihydro-8,9,13,24-tetramethyl- (9CI) (CA INDEX NAME)



L9 ANSWER 64 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1996:436548 CAPLUS  
 DOCUMENT NUMBER: 125:167644

ORIGINAL REFERENCE NO.: 125:31409a,31412a  
 TITLE: Versatile "3 + 1" syntheses of acenaphthoporphyrins, a new family of highly conjugated tetrapyrroles  
 AUTHOR(S): Chandrasekar, Pushpa; Lash, Timothy D.  
 CORPORATE SOURCE: Dep. Chem., Illinois State Univ., Normal, IL, 61790-4160, USA  
 SOURCE: Tetrahedron Letters (1996), 37(28), 4873-4876  
 CODEN: TELEAY; ISSN: 0040-4039  
 PUBLISHER: Elsevier  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 125:167644  
 GI

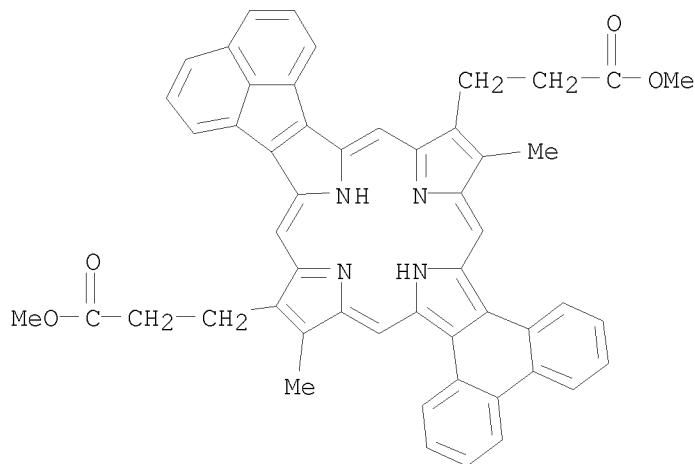


AB Acenaphthoporphyrins I (R = R1 = Et; RR1 = 1,8-naphthalenediyl, 1,1'-biphenyl-2,2'-diyl), a new group of porphyrins with strongly red shifted electronic absorption spectra, have been prepared by the acid catalyzed condensation of a pyrrole-2,5-dicarboxaldehyde with acenaphthotripyrranes; similarly, C-annelated pyrroledialdehydes afforded the related opp-diacenaphthoporphyrins and a mixed porphyrin system with fused phenanthrene and acenaphthylene rings.

IT 180199-09-1P  
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (versatile syntheses and electronic absorption spectra of acenaphthoporphyrins)

RN 180199-09-1 CAPLUS

CN 31H,33H-Acenaphtho[1,2-b]phenanthro[9,10-l]porphine-13,26-dipropanoic acid, 12,27-dimethyl-, dimethyl ester (9CI) (CA INDEX NAME)

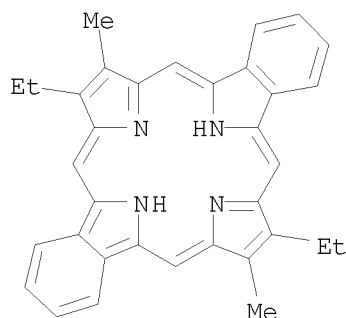


L9 ANSWER 65 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1996:418656 CAPLUS  
 DOCUMENT NUMBER: 125:109017  
 ORIGINAL REFERENCE NO.: 125:20315a,20318a  
 TITLE: Benzoporphyrins as photosensitizers for the photodynamic therapy of cancer  
 AUTHOR(S): Valles, Ma. Asuncion; Biolo, R.; Bonnett, Raymond; Canete, Magdalena; Gomez, Antonia Ma.; Jori, Giulio; Juarranz, Angeles; McManus, Kimberly A.; Okolo, Kawulia T.; et al.  
 CORPORATE SOURCE: Department de Quimica Organica, Universitat de Barcelona, Barcelona, 08028, Spain  
 SOURCE: Proceedings of SPIE-The International Society for Optical Engineering (1996), 2625(Photochemistry: Photodynamic Therapy and Other Modalities), 11-22  
 CODEN: PSISDG; ISSN: 0277-786X  
 PUBLISHER: SPIE-The International Society for Optical Engineering  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB A family of benzoporphyrins formed by differently substituted metallo tetrabenzoporphyrins and one opp-dibenzoporphyrin has been prepared The former benzoporphyrins, and meso-tetra(m-hydroxyphenyl)chlorin (m-THPC) to act as reference, have been encapsulated into liposomes and subjected to preliminary in vitro and in vivo assays to test their efficacy as photosensitizers in the photodynamic therapy of cancer. The results of the photocytotoxicity test shows that, with the exception of the nickel complexes 5, and 7/8, the other porphyrins are photobiol. active, the Mg-tetrabenzoporphyrin 1 and the opp-dibenzoporphyrin 10 being the most active. The dark toxicity of the photoactive porphyrins is in the range described for many photosensitizers, including HPD. The in vivo assays show no toxicity in the liver for any of the compds. tested, and also that 2 is the most promising photosensitizer among them, because of an efficient localization in an exptl. mouse tumor.  
 IT 81976-22-9  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(benzoporphyrins as photosensitizers for photodynamic therapy of cancer with red light)

RN 81976-22-9 CAPLUS

CN 25H,27H-Dibenzo[b,1]porphine, 8,20-diethyl-9,21-dimethyl- (9CI) (CA INDEX NAME)



L9 ANSWER 66 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1996:53078 CAPLUS

DOCUMENT NUMBER: 124:116939

ORIGINAL REFERENCE NO.: 124:21781a

TITLE: Simple Methodology for Syntheses of Porphyrins Possessing Multiple Peripheral Substituents with an Element of Symmetry

AUTHOR(S): Nguyen, Liem T.; Senge, Mathias O.; Smith, Kevin M.

CORPORATE SOURCE: Department of Chemistry, University of California, Davis, CA, 95616, USA

SOURCE: Journal of Organic Chemistry (1996), 61(3), 998-1003  
CODEN: JOCEAH; ISSN: 0022-3263

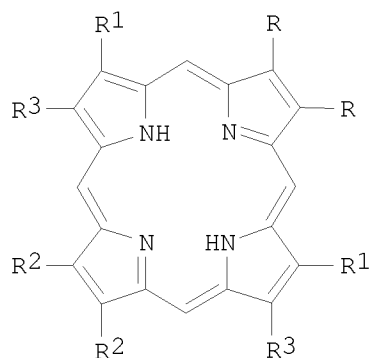
PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

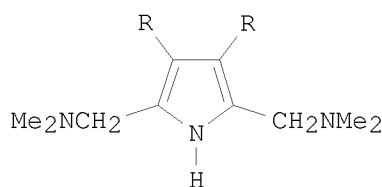
LANGUAGE: English

OTHER SOURCE(S): CASREACT 124:116939

GI



I



II

AB New methodol. was developed for synthesis of regiochem. pure porphyrins I



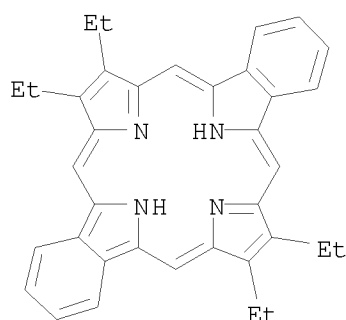
(R = R2 = Et; R1 = R3 = Me) with D2h symmetry via tetramerization reactions involving 3,4-dimethylpyrrole and II (R = Et). The corresponding opp-bis-benzoporphyrin was prepared by treatment with DDQ of I [R = R2 = (CH2)4; R1 = R3 = Et] from reaction of II (R = Et) and 4,5,6,7-tetrahydroisoindole. The synthetic method was further extended to allow the synthesis of more unsym. porphyrins I (R = Et; R1 = CH2CH2CO2Me; R2 = Ph; R3 = Me), with C2v symmetry, by reacting a tripyrrane with II (R = Ph). The structures and substituent arrays in both type of porphyrins were confirmed by single-crystal X-ray crystallog.

IT 160389-03-7P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(synthesis of sym. and unsym. porphyrins)

RN 160389-03-7 CAPLUS

CN 25H,27H-Dibenzo[b,l]porphine, 8,9,20,21-tetraethyl- (9CI) (CA INDEX NAME)



L9 ANSWER 67 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1996:14145 CAPLUS

DOCUMENT NUMBER: 124:116936

ORIGINAL REFERENCE NO.: 124:21777a,21780a

TITLE: Porphyrin synthesis by the "3 + 1" methodology: a superior approach for the preparation of porphyrins with fused 9,10-phenanthroline subunits

AUTHOR(S): Lin, Yanning; Lash, Timothy D.

CORPORATE SOURCE: Dep. Chem., Illinois State Univ., Normal, IL, 61790-4160, USA

SOURCE: Tetrahedron Letters (1995), 36(52), 9441-4

CODEN: TELEAY; ISSN: 0040-4039

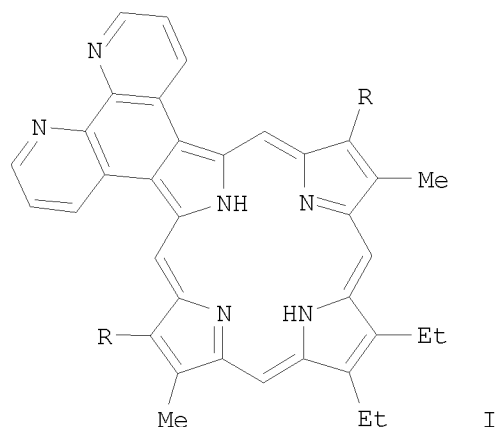
PUBLISHER: Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 124:116936

GI

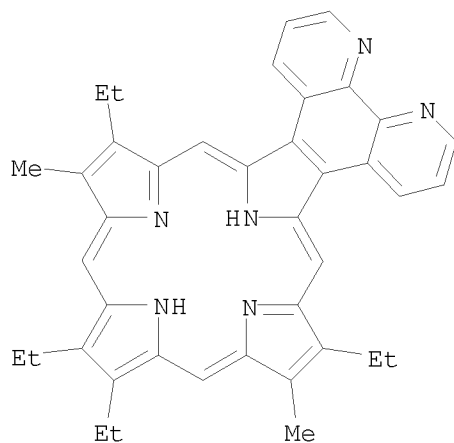


AB Porphyrins I (R = Et, Bu) with fused 1,10-phenanthroline subunits have been prepared in exceptionally high yields by the acid catalyzed condensation of phenanthroline substituted tripyrranes with a 2,5-pyrroledicarboxaldehyde.

IT 172806-00-7P 172806-03-0P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (phenanthrolineporphyrin synthesis via condensation of tripyrranes with pyrroledicarboxaldehyde)

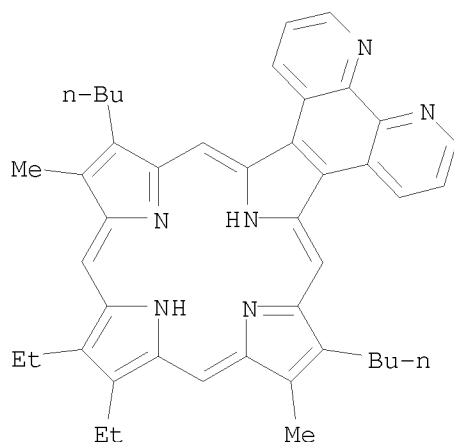
RN 172806-00-7 CAPLUS

CN 27H,29H-[1,10]Phenanthrolino[5,6-b]porphine,  
 12,17,18,23-tetraethyl-13,22-dimethyl- (9CI) (CA INDEX NAME)



RN 172806-03-0 CAPLUS

CN 27H,29H-[1,10]Phenanthrolino[5,6-b]porphine,  
 12,23-dibutyl-17,18-diethyl-13,22-dimethyl- (9CI) (CA INDEX NAME)



L9 ANSWER 68 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1995:874731 CAPLUS

DOCUMENT NUMBER: 123:266107

ORIGINAL REFERENCE NO.: 123:47393a, 47396a

TITLE: Pretargeting methods and compounds for pretargeted delivery of diagnostic and therapeutic agents

INVENTOR(S): Theodore, Louis J.; Meyer, Damon L.; Mallett, Robert W.; Kasina, Sudhakar; Reno, John M.; Axworthy, Donald B.; Gustavson, Linda M.

PATENT ASSIGNEE(S): Neorx Corp., USA

SOURCE: PCT Int. Appl., 250 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 14

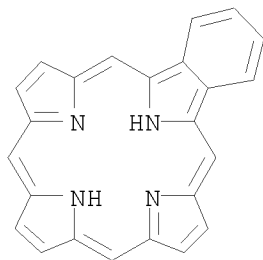
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9515979	A1	19950615	WO 1994-US14174	19941207
W: CA, JP				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
CA 2178476	A1	19950615	CA 1994-2178476	19941207
EP 733066	A1	19960925	EP 1995-905334	19941207
EP 733066	B1	20031119		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
JP 09506594	T	19970630	JP 1995-516363	19941207
EP 1346730	A1	20030924	EP 2003-8765	19941207
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE				
AT 254631	T	20031215	AT 1995-905334	19941207
PRIORITY APPLN. INFO.:				
			US 1993-163188	A 19931207
			EP 1995-905334	A3 19941207
			WO 1994-US14174	W 19941207

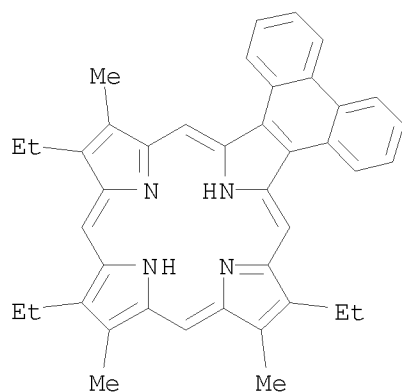
AB Methods, compds., compns. and kits that relate to pretargeted delivery of diagnostic and therapeutic agents are disclosed. Examples include e.g. in vivo anal. of a radiolabeled chelate-biotin conjugate administered after antibody pretargeting, clearing agent evaluation, two- and three-step

pretargeting methodol., and preparation of conjugates. The methodol. may also be used to increase photosensitizing agent localization.

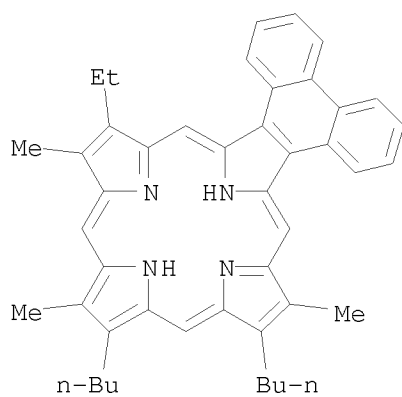
IT 36469-17-7D, 23H,25H-Benzo[b]porphine, derivs., conjugates with  
ligand/antiligand binding pair member  
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
(pretargeting methods and compds. for pretargeted delivery of  
diagnostic and therapeutic agents, and conjugate preparation)  
RN 36469-17-7 CAPLUS  
CN 23H,25H-Benzo[b]porphine (9CI) (CA INDEX NAME)



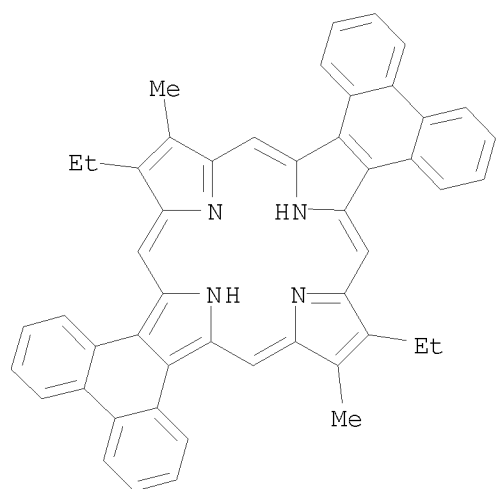
L9 ANSWER 69 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 1995:653749 CAPLUS  
DOCUMENT NUMBER: 123:83039  
ORIGINAL REFERENCE NO.: 123:14857a,14860a  
TITLE: New highly conjugated porphyrin chromophores:  
synthesis of mono- and diphenanthroporphyrins  
AUTHOR(S): Lash, Timothy D.; Novak, Bennett H.  
CORPORATE SOURCE: Dep. Chemistry, Illinois State Univ., Normal, IL,  
61790-4160, USA  
SOURCE: Tetrahedron Letters (1995), 36(25), 4381-84  
CODEN: TELEAY; ISSN: 0040-4039  
PUBLISHER: Elsevier  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 123:83039  
AB Porphyrins with one or two fused phenanthrene subunits have been prepared  
from phenanthro[9,10-c]pyrroles, which are in turn easily prepared from  
9-nitrophenanthrene.  
IT 165329-62-4P 165329-63-5P 165329-64-6P  
165329-65-7P 165329-66-8P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of mono- and diphenanthroporphyrins)  
RN 165329-62-4 CAPLUS  
CN 27H,29H-Phenanthro[9,10-b]porphine, 12,18,22-triethyl-13,17,23-trimethyl-  
(9CI) (CA INDEX NAME)



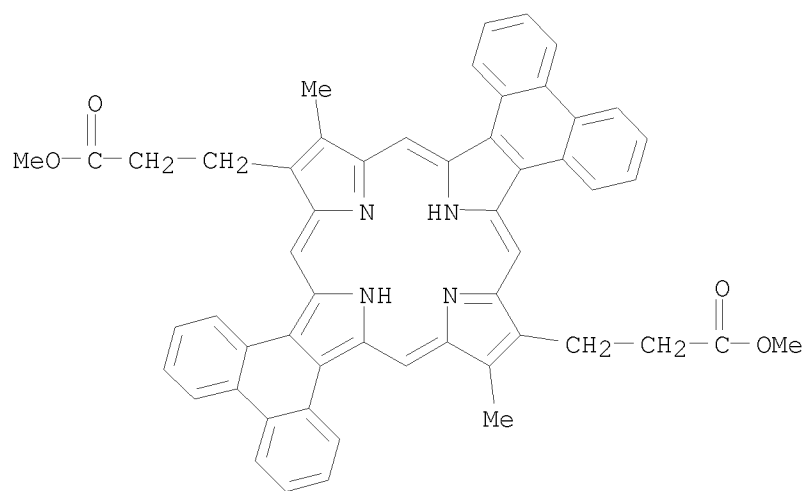
RN 165329-63-5 CAPLUS  
 CN 27H,29H-Phenanthro[9,10-b]porphine,  
 13,17-dibutyl-23-ethyl-12,18,22-trimethyl- (9CI) (CA INDEX NAME)



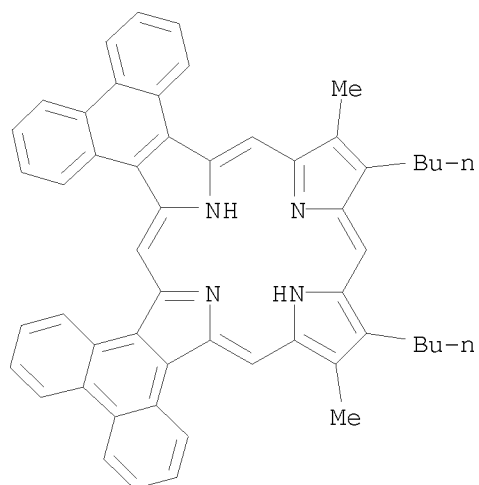
RN 165329-64-6 CAPLUS  
 CN 33H,35H-Diphenanthro[9,10-b:9',10'-l]porphine,  
 12,28-diethyl-13,29-dimethyl- (9CI) (CA INDEX NAME)



RN 165329-65-7 CAPLUS  
 CN 33H,35H-Diphenanthro[9,10-b:9',10'-l]porphine-12,28-dipropanoic acid,  
 13,29-dimethyl-, dimethyl ester (9CI) (CA INDEX NAME)



RN 165329-66-8 CAPLUS  
 CN 33H,35H-Diphenanthro[9,10-b:9',10'-g]porphine, 9,13-dibutyl-8,14-dimethyl-  
 (9CI) (CA INDEX NAME)



L9 ANSWER 70 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1995:323615 CAPLUS

DOCUMENT NUMBER: 122:160337

ORIGINAL REFERENCE NO.: 122:29545a,29548a

TITLE: Porphyrins with exocyclic rings. Part 5. Synthesis of naphtho[1,2-b]porphyrin

AUTHOR(S): Lash, Timothy D.; Denny, Carl P.

CORPORATE SOURCE: Dep. Chem., Illinois State Univ., Normal, IL, 61790-4160, USA

SOURCE: Tetrahedron (1995), 51(1), 59-66

CODEN: TETRAB; ISSN: 0040-4020

PUBLISHER: Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 122:160337

AB Condensation of 2-acetyl-1-tetralone with di-Et aminomalonate in refluxing acetic acid gave a dihydronaphthopyrrole in excellent yield. Transesterification with benzyl alc. gave the corresponding benzyl ester and subsequent regioselective oxidation with lead tetraacetate afforded the acetoxymethyl derivative This pyrrole was used in standard porphyrin chemical

to

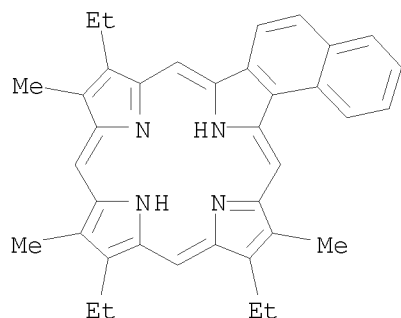
prepare 7,13,17-triethyl-8,12,18-trimethylnaphtho[1,2-b]porphyrin which exhibited an unusual electronic spectrum and this may have value in the characterization of sedimentary porphyrins.

IT 145179-53-9P

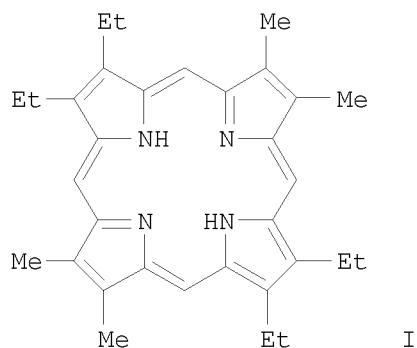
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and electronic spectrum of a naphtho[1,2-b]porphyrin)

RN 145179-53-9 CAPLUS

CN 25H,27H-Naphtho[1,2-b]porphine, 10,16,20-triethyl-11,15,21-trimethyl- (9CI) (CA INDEX NAME)



L9 ANSWER 71 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1995:248153 CAPLUS  
 DOCUMENT NUMBER: 122:80975  
 ORIGINAL REFERENCE NO.: 122:15383a,15386a  
 TITLE: One-pot synthesis of regiochemically pure porphyrins from two different pyrroles  
 AUTHOR(S): Nguyen, Liem T.; Senge, Mathias O.; Smith, Kevin M.  
 CORPORATE SOURCE: Dep. Chem., Univ. California, Davis, CA, 95616, USA  
 SOURCE: Tetrahedron Letters (1994), 35(41), 7581-4  
 CODEN: TELEAY; ISSN: 0040-4039  
 PUBLISHER: Elsevier  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 122:80975  
 GI

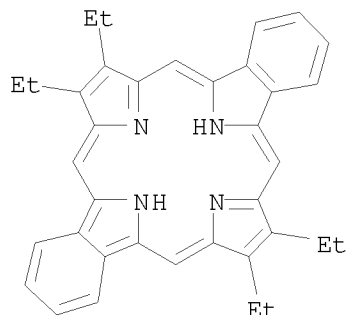


AB Treatment of 2,5-di-unsubstituted pyrroles, e.g., 3,4-diethylpyrrole, with excess of Eschenmoser's reagent (N,N-dimethylmethyleammonium iodide) affords 2,5-bis-(N,N-dimethylaminomethyl)pyrroles, e.g., 2,5-bis-(N,N-dimethylaminomethyl)-3,4-diethylpyrrole; reaction with a second 2,5-di-unsubstituted pyrrole, e.g., 3,4-dimethylpyrrole, gives pure porphyrin, e.g., I, with identical substituents on opposite pyrrole sub-units.

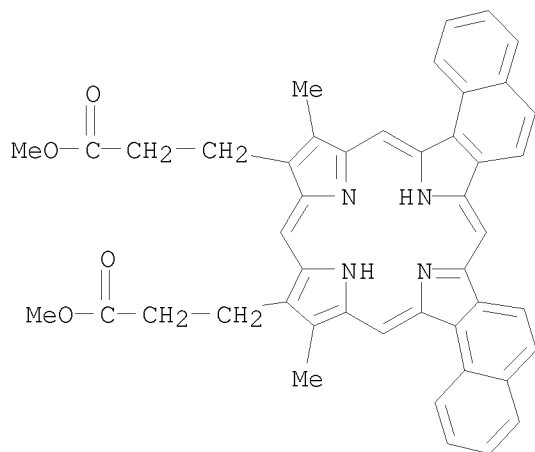
IT 160389-03-7P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of porphyrins with different pyrroles)



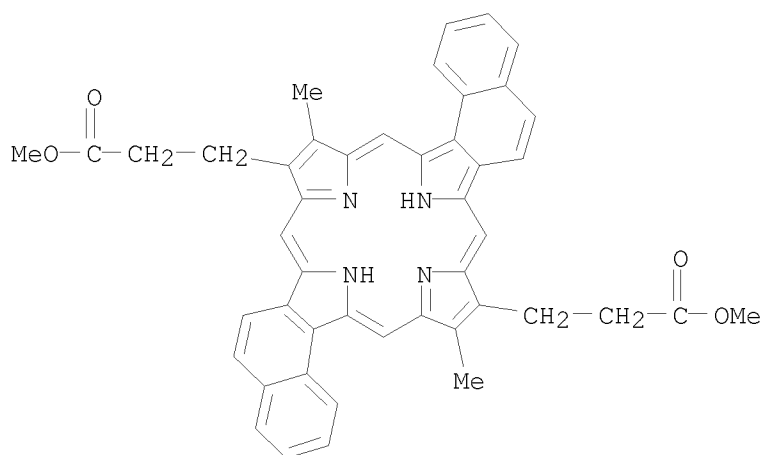
RN 160389-03-7 CAPLUS  
 CN 25H,27H-Dibenzo[b,1]porphine, 8,9,20,21-tetraethyl- (9CI) (CA INDEX NAME)



L9 ANSWER 72 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1995:141507 CAPLUS  
 DOCUMENT NUMBER: 122:9750  
 ORIGINAL REFERENCE NO.: 122:2169a,2172a  
 TITLE: Synthesis of dinaphthoporphyrins from  
 dihydronaphtho[1,2-c]pyrroles  
 AUTHOR(S): Lash, Timothy D.; Roper, Tracy J.  
 CORPORATE SOURCE: Dep. Chem., Illinois State Univ., Normal, IL,  
 61790-4160, USA  
 SOURCE: Tetrahedron Letters (1994), 35(42), 7715-18  
 CODEN: TELEAY; ISSN: 0040-4039  
 PUBLISHER: Elsevier  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Porphyrins with two fused dihydronaphtho units on the opposite or adjacent  
 adjacent pyrrole rings have been prepared by the MacDonald condensation or  
 by the cyclization of suitably substituted a,c-biladienes.  
 Dehydrogenation with 2 equiv of DDQ afforded the corresponding  
 dinaphthoporphyrins in excellent yields.  
 IT 159469-60-0P 159469-67-7P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (synthesis of dinaphthoporphyrins from dihydronaphtho[1,2-c]pyrroles)  
 RN 159469-60-0 CAPLUS  
 CN 29H,31H-Dinaphtho[1,2-b:2',1'-g]porphine-20,24-dipropenoic acid,  
 19,25-dimethyl-, dimethyl ester (9CI) (CA INDEX NAME)

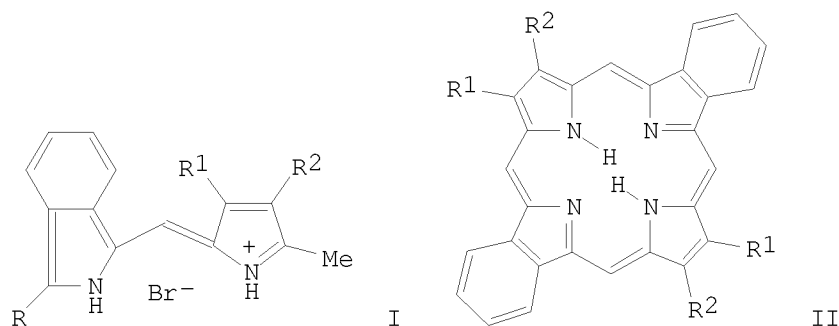


RN 159469-67-7 CAPLUS  
 CN 29H,31H-Dinaphtho[1,2-b:1',2'-1]porphine-10,24-dipropionic acid,  
 11,25-dimethyl-, dimethyl ester (9CI) (CA INDEX NAME)



L9 ANSWER 73 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1994:605066 CAPLUS  
 DOCUMENT NUMBER: 121:205066  
 ORIGINAL REFERENCE NO.: 121:37329a,37332a  
 TITLE: Opp-Dibenzoporphyrins from benzopyrromethene  
 derivatives  
 AUTHOR(S): Bonnett, Raymond; McManus, Kimberly A.  
 CORPORATE SOURCE: Chem. Dep., Queen Mary and Westfield Coll., London, E1  
 4NS, UK  
 SOURCE: Journal of the Chemical Society, Chemical  
 Communications (1994), (9), 1129-30  
 CODEN: JCCCAT; ISSN: 0022-4936  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

GI



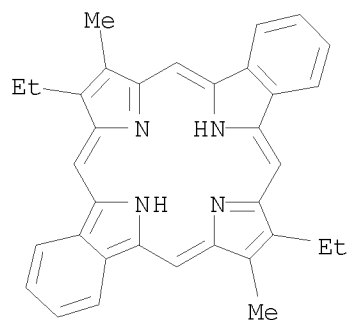
AB Condensation of 1-formyl-3-haloisoindoles with  $\alpha$ -free pyrroles in the presence of hydrogen bromide gives the corresponding benzopyrromethene hydrobromides. Heating  $\alpha$ -halo- $\alpha'$ -methylbenzopyrromethene hydrobromides I [R = Cl, R1 = Me, R2 = Et, H; R = Cl, R1 = Et, R2 = Me; R = Br, R1 = R2 = Me] in o-dichlorobenzene in air provides an economical synthesis of the opp-dibenzoporphyrin system II in acceptable yields.

IT 81976-22-9P 157869-31-3P 157869-32-4P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

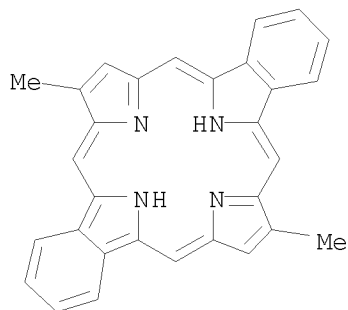
RN 81976-22-9 CAPLUS

CN 25H,27H-Dibenzo[b,1]porphine, 8,20-diethyl-9,21-dimethyl- (9CI) (CA INDEX NAME)

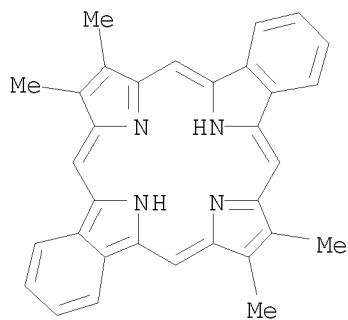


RN 157869-31-3 CAPLUS

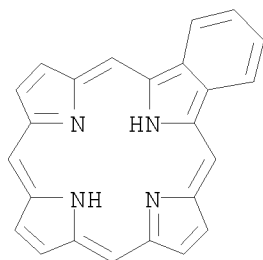
CN 25H,27H-Dibenzo[b,1]porphine, 8,20-dimethyl- (9CI) (CA INDEX NAME)



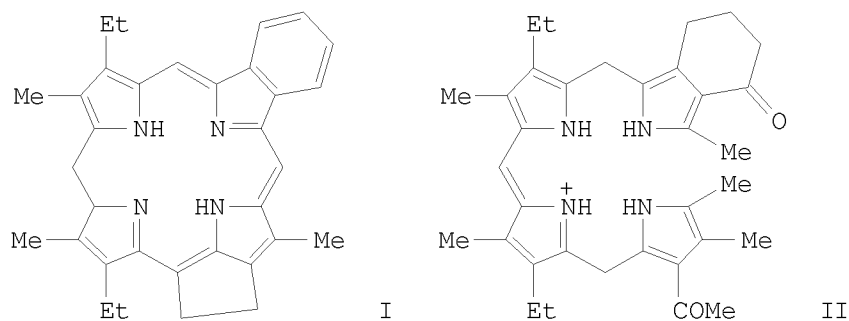
RN 157869-32-4 CAPLUS  
 CN 25H,27H-Dibenzo[b,l]porphine, 8,9,20,21-tetramethyl- (9CI) (CA INDEX NAME)



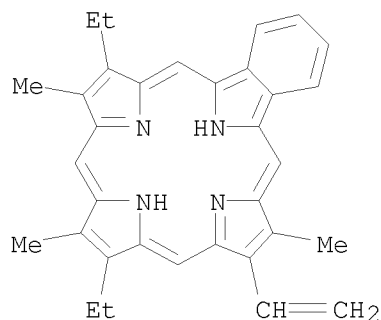
L9 ANSWER 74 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1994:453183 CAPLUS  
 DOCUMENT NUMBER: 121:53183  
 ORIGINAL REFERENCE NO.: 121:9511a,9514a  
 TITLE: Benzoporphyrin derivative and the photodynamic extracorporeal treatment of leukemia  
 AUTHOR(S): Jamieson, Catriona Helen Macleod  
 CORPORATE SOURCE: Univ. British Columbia, Vancouver, BC, Can.  
 SOURCE: (1992) 333 pp. Avail.: NLC, Order No. DANN79760  
 From: Diss. Abstr. Int. B 1993, 54(6), 2987  
 DOCUMENT TYPE: Dissertation  
 LANGUAGE: English  
 AB Unavailable  
 IT 36469-17-7D, 23H,25H-Benzo[b]porphine, derivative  
 RL: BIOL (Biological study)  
 (photodynamic extracorporeal treatment of leukemia with)  
 RN 36469-17-7 CAPLUS  
 CN 23H,25H-Benzo[b]porphine (9CI) (CA INDEX NAME)



L9 ANSWER 75 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1994:323036 CAPLUS  
 DOCUMENT NUMBER: 120:323036  
 ORIGINAL REFERENCE NO.: 120:56821a,56824a  
 TITLE: The chemistry of pyrrolic compounds. LXIX. A synthesis of one of the naturally occurring benzoporphyrins  
 AUTHOR(S): Clezy, Peter S.; Leung, Christopher W. F.  
 CORPORATE SOURCE: Dep. Org. Chem., Univ. New South Wales, Kensington, 2033, Australia  
 SOURCE: Australian Journal of Chemistry (1993), 46(11), 1705-10  
 CODEN: AJCHAS; ISSN: 0004-9425  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



AB The naturally occurring benzoporphyrin I has been prepared by ring synthesis utilizing an oxidative cyclization of an intermediate bilene-bilene II to assemble the porphyrin macrocycle.  
 IT 155127-29-0  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (intermediate, synthesis of benzoporphyrin)  
 RN 155127-29-0 CAPLUS  
 CN 23H,25H-Benzo[b]porphine, 9-ethenyl-13,19-diethyl-8,14,18-trimethyl- (9CI)  
 (CA INDEX NAME)



L9 ANSWER 76 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1994:293146 CAPLUS

DOCUMENT NUMBER: 120:293146

ORIGINAL REFERENCE NO.: 120:51526h, 51527a

TITLE: Transcutaneous in vivo activation of photosensitive agents in blood

INVENTOR(S): Richter, Anna M.

PATENT ASSIGNEE(S): Quadra Logic Technologies, Inc., Can.

SOURCE: PCT Int. Appl., 45 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9406424	A1	19940331	WO 1993-CA382	19930920
W: AT, AU, BB, BG, BR, BY, CA, CH, CZ, DE, DK, ES, FI, GB, HU, JP, KP, KR, KZ, LK, LU, MG, MN, MW, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SK, UA, VN				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9349405	A	19940412	AU 1993-49405	19930920
AU 681088	B2	19970821		
EP 660712	A1	19950705	EP 1993-918860	19930920
EP 660712	B1	20010530		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
HU 70966	A2	19951128	HU 1995-814	19930920
HU 220251	B	20011128		
JP 08501301	T	19960213	JP 1994-507629	19930920
JP 3598306	B2	20041208		
IL 107035	A	19981227	IL 1993-107035	19930920
NZ 255302	A	20010427	NZ 1993-255302	19930920
JP 2001316288	A	20011113	JP 2001-105544	19930920
ES 2160600	T3	20011116	ES 1993-918860	19930920
PT 660712	T	20011130	PT 1993-918860	19930920
CA 2144327	C	20020806	CA 1993-2144327	19930920
ZA 9306968	A	19940412	ZA 1993-6968	19930921
US 5484803	A	19960116	US 1995-384440	19950202
FI 9501295	A	19950517	FI 1995-1295	19950320
NO 9501066	A	19950519	NO 1995-1066	19950320

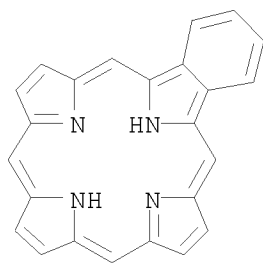
US 5736563	A	19980407	US 1995-555235	19951108
GR 3036479	T3	20011130	GR 2001-401338	20010830
PRIORITY APPLN. INFO.:			US 1992-948113	A 19920921
			JP 1994-507629	A3 19930920
			WO 1993-CA382	W 19930920
			US 1995-384440	A1 19950202

AB A method is disclosed that destroys or impairs target cells that have selectively accumulated a photosensitizing agent. The target cells are in the bloodstream of an intact animal, which bloodstream and animal further contain nontarget cells. Radiation is applied transcutaneously to at least a portion of the intact animal at an intensity effective to impair or destroy selectively the target cells and to leave nontarget cells relatively unimpaired. Target cells include leukemia cells, virus-containing cells, parasite-containing cells, and microorganisms (e.g. bacteria, parasites, free viruses). Results of animal studies showed that whole-body exposure to red light, following injection of BPD (benzoporphyrin derivs.), caused activation of BPD in the blood. As a result some of the BPD was photodegraded and, at the same time, a large number of BPD-preloaded tumor cells were destroyed. After treatment, neither skin photosensitivity nor change in the behavior of the animals was observed (maximum observation period was 2 wk).

IT 36469-17-7D, 23H,25H-Benzo[b]porphine, monocarboxylated and other derivs.  
 RL: BIOL (Biological study)  
 (transcutaneous radiation and bloodstream-contained cells with, for target cell destruction)

RN 36469-17-7 CAPLUS

CN 23H,25H-Benzo[b]porphine (9CI) (CA INDEX NAME)



L9 ANSWER 77 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1994:293144 CAPLUS

DOCUMENT NUMBER: 120:293144

ORIGINAL REFERENCE NO.: 120:51523a,51526a

TITLE: Method for destroying or inhibiting growth of unwanted cells or tissues using benzoporphyrin derivative photosensitizers and ionizing radiation

INVENTOR(S): Richter, Anna; Levy, Julia G.; Dolphin, David

PATENT ASSIGNEE(S): Quadra Logic Technologies, Inc., Can.

SOURCE: PCT Int. Appl., 36 pp.  
 CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9404147	A1	19940303	WO 1993-CA328	19930817
W: AU, CA, DK, FI, JP, KR, NO, SE				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
AU 9346954	A	19940315	AU 1993-46954	19930817
EP 654993	A1	19950531	EP 1993-917495	19930817
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
JP 08505361	T	19960611	JP 1994-505711	19930817
CN 1099612	A	19950308	CN 1993-116757	19930903
NO 9500610	A	19950316	NO 1995-610	19950217
FI 9500730	A	19950410	FI 1995-730	19950217
US 5945439	A	19990831	US 1997-887087	19970702
PRIORITY APPLN. INFO.:			US 1992-930165	A 19920817
			WO 1993-CA328	W 19930817

OTHER SOURCE(S): MARPAT 120:293144

AB A process is disclosed for the use of a combination of ionizing radiation in conjunction with certain benzoporphyrin derivative compds. (BPD), preferably the compound benzoporphyrin derivative-monoacid ring-A (BPD-MA), to mediate the destruction of diseased or unwanted cells or tissues. Specifically, the invention is a method in which the sensitizer compds. are administered either systemically or locally to the diseased or unwanted tissue and irradiated with ionizing radiation (from e.g. <sup>60</sup>Co or x-rays). The treatment with benzoporphyrin derivative compds. appears to sensitize the target cells or tissues in that those cells do not readily recover from irradiation exposure. Addnl., the process may be used to lower the effective amount of radiation applied to a particular tissue target. The effect of BPD-MA and radiation in tumor-bearing mice is described.

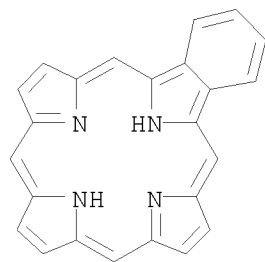
IT 36469-17-7D, 23H,25H-Benzo[b]porphine, monocarboxylated and other derivs.

RL: BIOL (Biological study)

(ionizing radiation and radiosensitizer of, for unwanted cell or tissue destruction)

RN 36469-17-7 CAPLUS

CN 23H,25H-Benzo[b]porphine (9CI) (CA INDEX NAME)



L9 ANSWER 78 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1994:100742 CAPLUS

DOCUMENT NUMBER: 120:100742

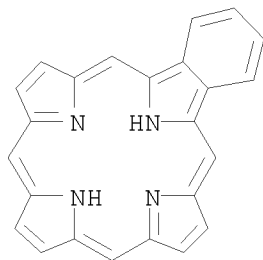
ORIGINAL REFERENCE NO.: 120:17726h,17727a

TITLE: The effect of differentiation of photosensitizer uptake by HL60 cells

AUTHOR(S): Korbelyik, Mladen; Krosi, Gorazd; Adomat, Hans; Skov,



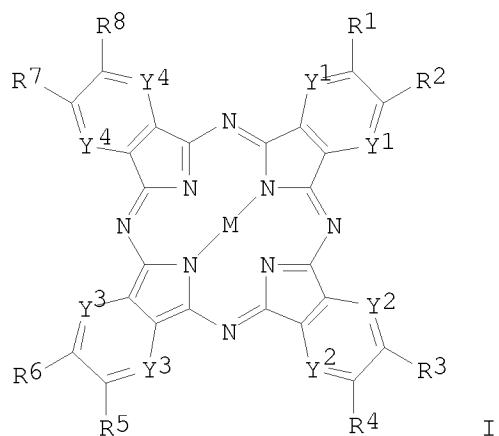
Kristen A.  
CORPORATE SOURCE: Cancer Imaging, BC Cancer Res. Cent., Vancouver, BC, V5Z 1L3, Can.  
SOURCE: Photochemistry and Photobiology (1993), 58(5), 670-5  
CODEN: PHCBAP; ISSN: 0031-8655  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB The capability of human promyelocytic leukemia cells HL60 to be induced to differentiate to various stages along the monocytic or myelocytic pathway was exploited for investigation of the uptake of selected photosensitizers by diverse types of cells of the same origin. The results showed that there was no substantial difference in Photofrin uptake between noninduced HL60 cells, immature monocytes, immature neutrophils and cells differentiated along the eosinophilic pathway. In contrast, HL60 cells differentiated into macrophages (HL60Φ) exhibited markedly increased Photofrin uptake, which was further enhanced by their pretreatment with bacterial lipopolysaccharide. Similar results were obtained with other photosensitizers tested: di- and tetrasulfonated aluminum phthalocyanines (AlPcS2 and AlPcS4), tetrasulfonated zinc phthalocyanine (ZnPcS4), tetraphenylporphine tetrasulfonate (TPPS4) and benzoporphyrin derivative monoacid (BPD). Despite marked differences in the state of self-aggregation and other chemical properties of these compds., the degree of their preferential uptake by HL60Φ cells showed very little variation. In a typical experiment, the uptake of these photosensitizers by HL60Φ cells was 4-5-fold higher than the uptake by noninduced HL60 cells. In addition to the fluorometric assay employed in most of the expts., the cellular concentration of AlPcS was determined by measurement of elementary aluminum using atomic absorption spectroscopy.  
IT 36469-17-7D, 23H,25H-Benzo[b]porphine, derivs.  
RL: BIOL (Biological study)  
(uptake of, by human promyelocytic leukemia cells, differentiation effect on)  
RN 36469-17-7 CAPLUS  
CN 23H,25H-Benzo[b]porphine (9CI) (CA INDEX NAME)



L9 ANSWER 79 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 1993:182184 CAPLUS  
DOCUMENT NUMBER: 118:182184  
ORIGINAL REFERENCE NO.: 118:30980h,30981a  
TITLE: Benzopyrazinoporphyrazine derivatives with near-infrared absorption  
INVENTOR(S): Tokita, Sumio  
PATENT ASSIGNEE(S): Nippon Soda Co., Ltd., Japan  
SOURCE: Jpn. Kokai Tokkyo Koho, 7 pp.

CODEN: JKXXAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 04283581	A	19921008	JP 1991-72063	19910313
PRIORITY APPLN. INFO.:			JP 1991-72063	19910313
OTHER SOURCE(S):	MARPAT	118:182184		
GI				



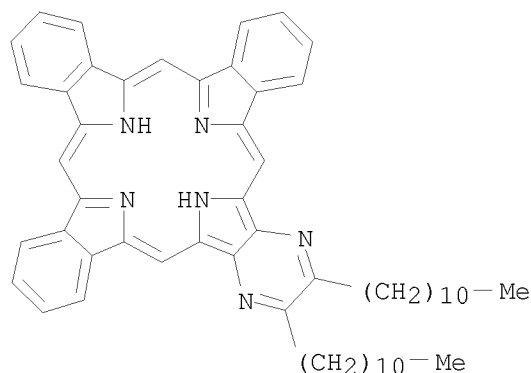
AB The title derivs. I [R1-8 = X1[(CH2)mX2]nR9; X1 = CH2, O, S, NR10; X2 = O, S, NR11; R9-11 = (un)substituted alkyl, aryl, or alkenyl; Y1-4 = N, CH; not all of Y1-4 are the same; M = 2H, metal, metal oxide, metal hydroxide, acyl metal, metal alkoxide, metal siloxide, metal halide; m,n = 0-3] are claimed. I, with high near-IR absorption and organic solvent solubility, are useful for optical recording media, electrophotog. photoreceptors, redox catalysts, flower preservatives, etc.

IT 146628-43-5P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of, near-IR-absorbing)

RN 146628-43-5 CAPLUS

CN 29H,31H-Tribenzo[b,g,l]pyrazino[2,3-q]porphine, 2,3-diundecyl- (9CI) (CA INDEX NAME)



L9 ANSWER 80 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1993:127825 CAPLUS

DOCUMENT NUMBER: 118:127825

ORIGINAL REFERENCE NO.: 118:22091a,22094a

TITLE: Geochemical origins of sedimentary benzoporphyrins and tetrahydrobenzoporphyrins

AUTHOR(S): Lash, Timothy D.

CORPORATE SOURCE: Dep. Chem., Illinois State Univ., Normal, IL, 61761-6901, USA

SOURCE: Energy & Fuels (1993), 7(2), 166-71

CODEN: ENFUEM; ISSN: 0887-0624

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Complex mixts. of metalloporphyrins are associated with organic-rich sediments. Although some of these petroporphyrins were correlated with known biol. pigments, the origins of certain structures are obscure. Benzoporphyrins and tetrahydrobenzoporphyrins, 2 minor families of geol. tetrapyrroles, were isolated from numerous oil shales and petroleums but the origins of these mol. fossils are poorly understood. A number of possible pathways for the geochem. formation of benzo- and tetrahydrobenzoporphyrins are discussed. The data presently available favors a Diels-Alder cycloaddn. mechanism between putative divinylchlorophyll and quinone precursors for the formation of these compds. As an aid to these studies, total syntheses of benzo- and naphthoporphyrins were been carried out and the spectroscopic properties of these extended chromophores are discussed. Further studies are proposed to help distinguish between the various possible pathways for the geochem. genesis of tetrahydrobenzo- and benzoporphyrins.

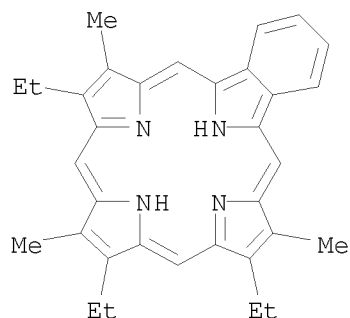
IT 145179-52-8P 145179-53-9P

RL: PREP (Preparation)

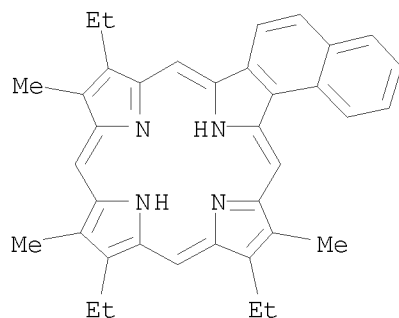
(preparation of, geochem. origins of sedimentary benzoporphyrins and tetrahydrobenzoporphyrins in relation to)

RN 145179-52-8 CAPLUS

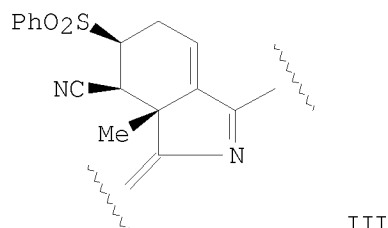
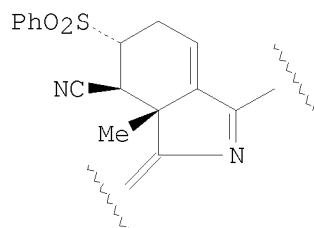
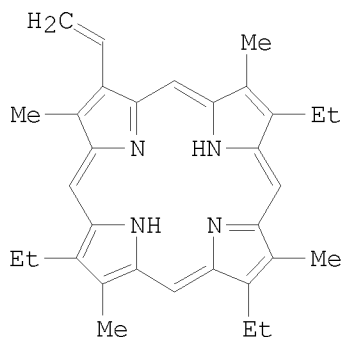
CN 23H,25H-Benzo[b]porphine, 9,13,18-triethyl-8,14,19-trimethyl- (9CI) (CA INDEX NAME)



RN 145179-53-9 CAPLUS  
 CN 25H,27H-Naphtho[1,2-b]porphine, 10,16,20-triethyl-11,15,21-trimethyl-  
 (9CI) (CA INDEX NAME)



L9 ANSWER 81 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1992:633672 CAPLUS  
 DOCUMENT NUMBER: 117:233672  
 ORIGINAL REFERENCE NO.: 117:40399a,40402a  
 TITLE: Regioselective and stereoselective Diels-Alder reactions of unsymmetrical 1,2-disubstituted vinyl sulfones with monovinylporphyrin  
 AUTHOR(S): Yon-Hin, Paul; Wijesekera, Tilak P.; Dolphin, David  
 CORPORATE SOURCE: Dep. Chem., Univ. British Columbia, Vancouver, BC, V6T 1Y6, Can.  
 SOURCE: New Journal of Chemistry (1992), 16(5), 537-9  
 CODEN: NJCHE5; ISSN: 1144-0546  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 117:233672  
 GI



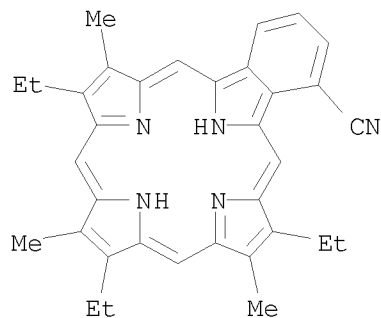
AB A study of the Diels-Alder reactions of several 1,2-disubstituted vinyl sulfones with a  $\beta$ -methyl- $\beta'$ -monovinylporphyrin (I) shows that the cycloaddns. are highly regioselective and that stereochem. control can be manipulated by replacing a carboxyl ester group by a cyano group or by changing of the dienophile. Thus, reacting I with (E)- and (Z)-PhSO<sub>2</sub>CH:CHCN gave adducts II and III, resp.

IT 144460-87-7P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 144460-87-7 CAPLUS

CN 23H,25H-Benzo[b]porphine-1-carbonitrile,  
9,14,19-triethyl-8,13,18-trimethyl- (9CI) (CA INDEX NAME)



L9 ANSWER 82 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1992:238486 CAPLUS

DOCUMENT NUMBER: 116:238486

ORIGINAL REFERENCE NO.: 116:40381a,40384a

TITLE: Biological markers in Chinese ancient sediments. 1. Geoporphyrins

AUTHOR(S): Peng, Pingan; Eglinton, G.; Fu, Jiamo; Sheng, Guoying

CORPORATE SOURCE: Sch. Chem., Univ. Bristol, Bristol, BS8 1TS, UK

SOURCE: Energy & Fuels (1992), 6(2), 215-25  
CODEN: ENFUEM; ISSN: 0887-0624

DOCUMENT TYPE: Journal

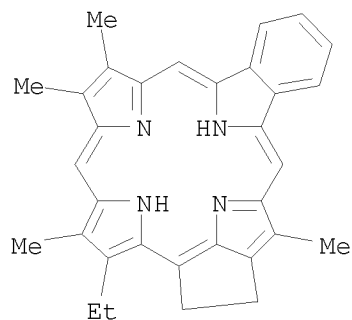
LANGUAGE: English

AB Eleven Chinese ancient sediments (9 Paleocene and 2 Permian) from freshwater lacustrine, hypersaline lacustrine, coal swamp, and marine deposits (4, 4, 2, and 1 samples, resp.) were examined for content and distribution of geoporphyrins and compared with those of 3 reference samples [e.g., Gilsonite bitumen (saline lacustrine), Serpiano oil shale (marine anoxic), and Boscan oil (marine anoxic)]. The geoporphyrins were isolated as sep. Ni and vanadyl fractions. Demetallation afforded free geoporphyrins which were examined by HPLC (normal phase with silica); the HPLC traces could be grouped into 4 different paleoenvironmental types. Assignments of .apprx.15 major porphyrins could be made by coinjection of porphyrin stds. isolated from the reference samples. Conversion of free base porphyrins to their bis(tert-butyldimethyl)silyl derivs., followed by gas chromatog.-mass spectroscopy (GC-MS) and computerized data processing, provided the distributions of 38 compds., which were also assigned by coinjection of stds. These 38 compds. (in 8 series) account for 49-85% of total porphyrins (mostly >70%). A series of 4 unidentified geoporphyrins is dominant in samples from hypersaline lacustrine paleoenvironments. These compds. coelute with 131-Me cycloalkylporphyrins on normal-phase HPLC but are clearly separable on GC-MS.

IT 100813-32-9  
RL: OCCU (Occurrence)  
(biomarker, in ancient geol. sediments, of China)

RN 100813-32-9 CAPLUS

CN 5,22:12,15-Diimino-20,18-metheno-7,10-nitrilobenzo[o]cyclopent[b]azacyclononadecine, 14-ethyl-16,17-dihydro-8,9,13,24-tetramethyl- (9CI) (CA INDEX NAME)



L9 ANSWER 83 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1992:190223 CAPLUS

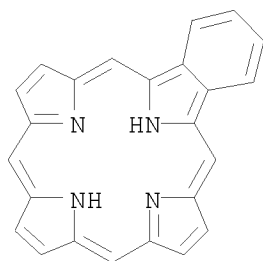
DOCUMENT NUMBER: 116:190223

ORIGINAL REFERENCE NO.: 116:32119a,32122a

TITLE: Photosensitizing potency of structural analogs of benzoporphyrin derivative (BPD) in a mouse tumor model

AUTHOR(S): Richter, A. M.; Waterfield, E.; Jain, A. K.; Allison,

CORPORATE SOURCE: B.; Sternberg, E. D.; Dolphin, D.; Levy, J. G.  
 Dep. Microbiol., Univ. British Columbia, Vancouver,  
 BC, V6T 1W5, Can.  
 SOURCE: British Journal of Cancer (1991), 63(1), 87-93  
 CODEN: BJCAAI; ISSN: 0007-0920  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB The in vivo characteristics of four analogs of benzoporphyrin derivative (BPD) were investigated. Biodistribution data obtained in DBA/2J mice with BPD-MA (monoacid ring A analog) which had been tritiated or internally labeled with <sup>14</sup>C showed that both labeled materials acted in an essentially identical manner during the period of study. Biodistribution and clearance studies showed that relative distribution in a variety of mouse tissues was similar for all BPD analogs. M 1 tumor cells (rhabdomyosarcoma in DBA/2J mice) taken from tumors excised from animals treated 3 h earlier with BPD, and tested in vitro for photosensitivity provided evidence that significant levels of photosensitizer detected in tumor was both active and associated with tumor cells. The monoacid forms of BPD were found to be much more photodynamically active in this test were the diacid analogs. The ability of the analogs to ablate tumors in mice by photodynamic therapy was also tested. Again, BPD-MA and BPD-MB proved to be measurably better than the diacid analogs. These findings are discussed in reference to structural and phys. differences between the analogs.  
 IT 36469-17-7D, 23H,25H-Benzo[b]porphine, derivs.  
 RL: BIOL (Biological study)  
 (36469177)  
 RN 36469-17-7 CAPLUS  
 CN 23H,25H-Benzo[b]porphine (9CI) (CA INDEX NAME)



L9 ANSWER 84 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1991:549231 CAPLUS  
 DOCUMENT NUMBER: 115:149231  
 ORIGINAL REFERENCE NO.: 115:25321a,25324a  
 TITLE: Tabulation of exact masses and comparison of isotope patterns expected for geoporphyrin molecular ions in electron ionization mass spectra  
 AUTHOR(S): Van Berkel, Gary J.; Castro, Aidalu Joubert; Filby, Royston H.  
 CORPORATE SOURCE: Anal. Chem. Div., Oak Ridge Natl. Lab., Oak Ridge, TN, 37831-6365, USA  
 SOURCE: Applied Geochemistry (1991), 6(1), 105-17  
 CODEN: APPGEY; ISSN: 0883-2927  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB Exact masses ( $\pm 0.0001$  u) were tabulated (Cmin-C50) for free-base, Mn, Fe, Ni, Cu, Zn, vanadyl (VO), and Ga complexes of the major geoporphyrin skeletal types and several com. available porphyrin complexes. The data in these tables are intended as a resource to aid in geoporphyrin identification (i.e. determination of carbon number, skeletal type and metal chelated) by low-resolution electron ionization-mass spectrometry (EI-MS) and by high-resolution EI-MS in cases where exact mass determination is performed.

A comparison was made of the isotope patterns calculated for the mol. ions of the various porphyrin skeletal types as free-base species and as the 7 metal complexes mentioned above. The isotope pattern of a metalloporphyrin mol. ion is a useful aid in identifying the metal complexed. Correction of mol. ion abundances (i.e. porphyrin abundances) for overlap of mol. ion isotope peaks and for overlap of fragment ion peaks with mol. ion peaks, both of which can occur when analyzing complex geoporphyrin mixts., is discussed.

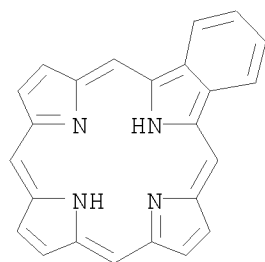
IT 36469-17-7D, 23H,25H-Benzo[b]porphine, alkyl derivs.  
 99625-79-3D, alkyl derivs. 128920-36-5D, alkyl derivs.  
 135539-74-1D, alkyl derivs. 135539-75-2D, alkyl derivs.  
 135539-76-3D, alkyl derivs. 135539-77-4D, alkyl derivs.  
 135539-78-5D, alkyl derivs. 135539-79-6D, alkyl derivs.  
 135539-80-9D, alkyl derivs. 135539-81-0D, alkyl derivs.  
 135539-82-1D, alkyl derivs. 135539-83-2D, alkyl derivs.  
 135539-84-3D, alkyl derivs. 135539-85-4D, alkyl derivs.  
 135539-86-5D, alkyl derivs.

RL: ANT (Analyte); ANST (Analytical study)

(identification of, by mass spectroscopy, exact mass calcns. for)

RN 36469-17-7 CAPLUS

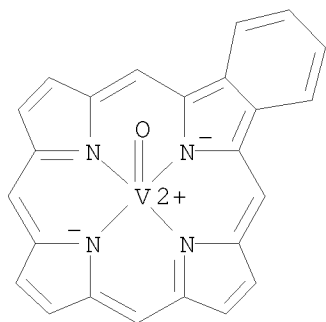
CN 23H,25H-Benzo[b]porphine (9CI) (CA INDEX NAME)



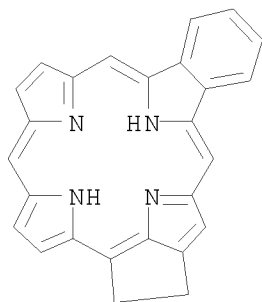
RN 99625-79-3 CAPLUS

CN Vanadium, [23H,25H-benzo[b]porphinato(2-)-N23,N24,N25,N26]oxo-, (SP-5-12)-  
 (9CI) (CA INDEX NAME)

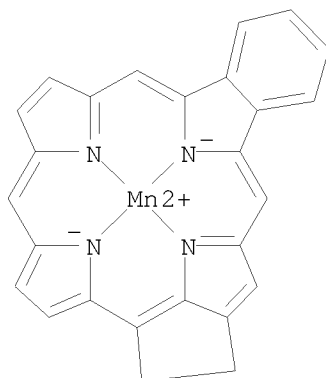




RN 128920-36-5 CAPLUS  
 CN 5,22:12,15-Diimino-20,18-metheno-7,10-nitrilobenzo[o]cyclopent[b]azacyclononadecine, 16,17-dihydro- (9CI) (CA INDEX NAME)

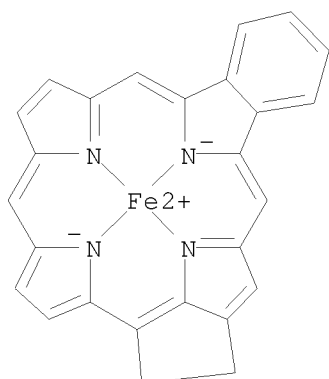


RN 135539-74-1 CAPLUS  
 CN Manganese, [16,17-dihydro-5,22:12,15-diimino-20,18-metheno-7,10-nitrilobenzo[o]cyclopent[b]azacyclononadecinato(2-)-N19,N23,N25,N26]-, (SP-4-2)- (9CI) (CA INDEX NAME)



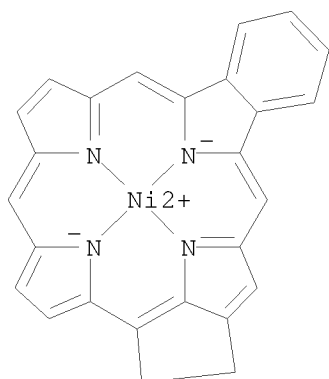
RN 135539-75-2 CAPLUS  
 CN Iron, [16,17-dihydro-5,22:12,15-diimino-20,18-metheno-7,10-nitrilobenzo[o]cyclopent[b]azacyclononadecinato(2-)-N19,N23,N25,N26]-,

(SP-4-2)- (9CI) (CA INDEX NAME)



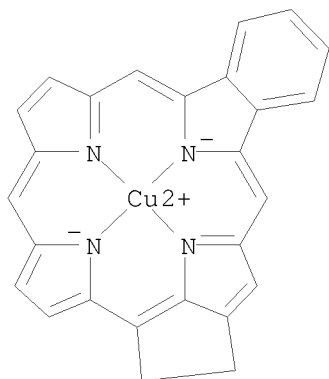
RN 135539-76-3 CAPLUS

CN Nickel, [16,17-dihydro-5,22:12,15-diimino-20,18-metheno-7,10-nitrilobenzo[o]cyclopent[b]azacyclononadecinato(2-)-N19,N23,N25,N26]-, (SP-4-2)- (9CI) (CA INDEX NAME)



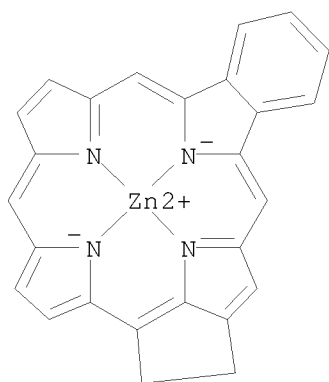
RN 135539-77-4 CAPLUS

CN Copper, [16,17-dihydro-5,22:12,15-diimino-20,18-metheno-7,10-nitrilobenzo[o]cyclopent[b]azacyclononadecinato(2-)-N19,N23,N25,N26]-, (SP-4-2)- (9CI) (CA INDEX NAME)



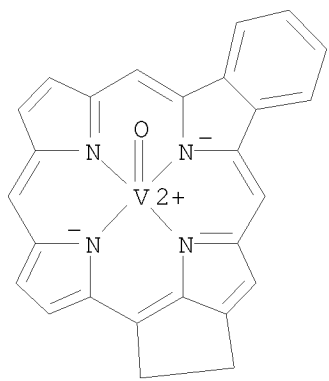
RN 135539-78-5 CAPLUS

CN Zinc, [16,17-dihydro-5,22:12,15-diimino-20,18-metheno-7,10-nitrilobenzo[o]cyclopent[b]azacyclononadecinato(2-)-N19,N23,N25,N26]-, (SP-4-2)- (9CI) (CA INDEX NAME)



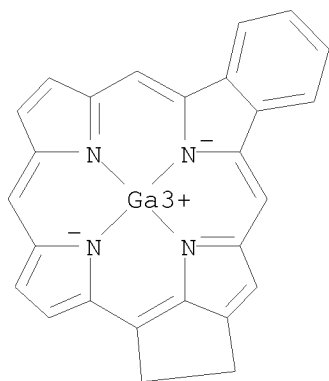
RN 135539-79-6 CAPLUS

CN Vanadium, [16,17-dihydro-5,22:12,15-diimino-20,18-metheno-7,10-nitrilobenzo[o]cyclopent[b]azacyclononadecinato(2-)-N19,N23,N25,N26]oxo-, (SP-5-13)- (9CI) (CA INDEX NAME)



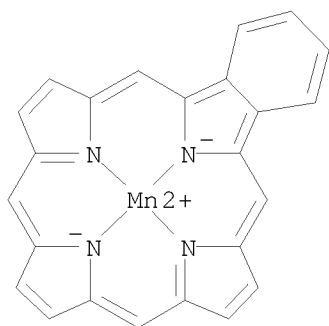
RN 135539-80-9 CAPLUS

CN Gallium(1+), [16,17-dihydro-5,22:12,15-diimino-20,18-metheno-7,10-nitrilobenzo[o]cyclopent[b]azacyclononadecinato(2-)-N19,N23,N25,N26]-, (SP-4-2)- (9CI) (CA INDEX NAME)



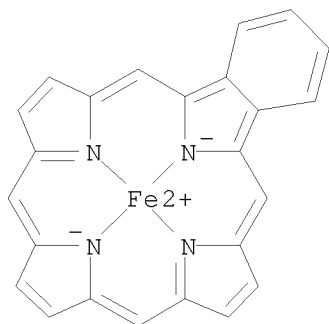
RN 135539-81-0 CAPLUS

CN Manganese, [23H,25H-benzo[b]porphinato(2-)-N23,N24,N25,N26]-, (SP-4-1)- (9CI) (CA INDEX NAME)

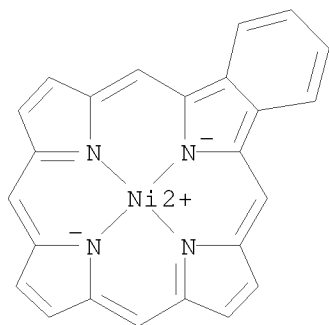


RN 135539-82-1 CAPLUS

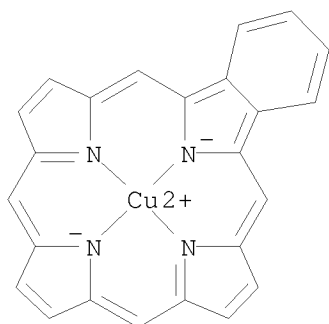
CN Iron, [23H,25H-benzo[b]porphinato(2-)-N23,N24,N25,N26]- (9CI) (CA INDEX NAME)



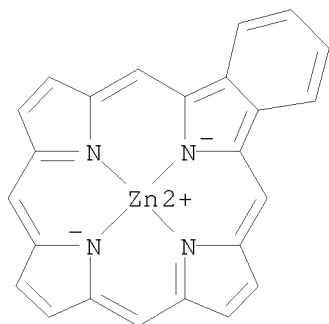
RN 135539-83-2 CAPLUS  
 CN Nickel, [23H,25H-benzo[b]porphinato(2-)-N23,N24,N25,N26]-, (SP-4-1)- (9CI)  
 (CA INDEX NAME)



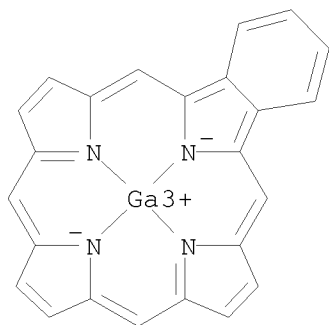
RN 135539-84-3 CAPLUS  
 CN Copper, [23H,25H-benzo[b]porphinato(2-)-N23,N24,N25,N26]-, (SP-4-1)- (9CI)  
 (CA INDEX NAME)



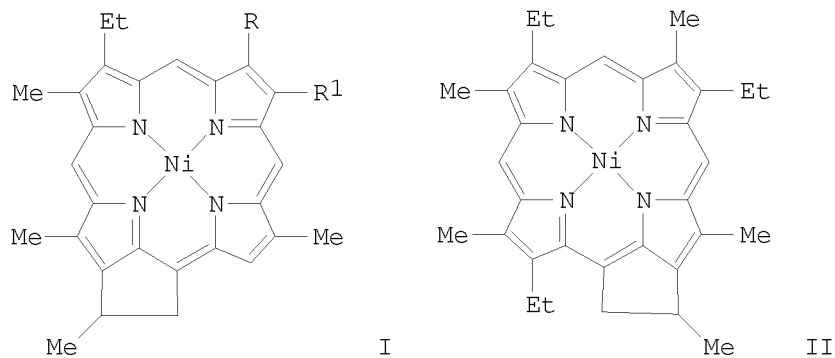
RN 135539-85-4 CAPLUS  
 CN Zinc, [23H,25H-benzo[b]porphinato(2-)-N23,N24,N25,N26]-, (SP-4-1)- (9CI)  
 (CA INDEX NAME)



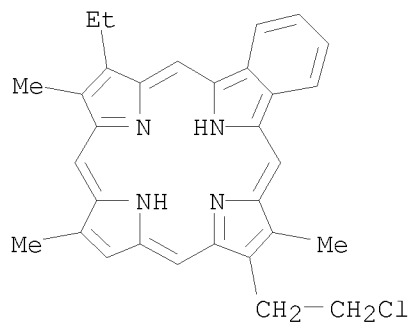
RN 135539-86-5 CAPLUS  
 CN Gallium(1+), [23H,25H-benzo[b]porphinato(2-)-N23,N24,N25,N26]-, (SP-4-1)-  
 (9CI) (CA INDEX NAME)



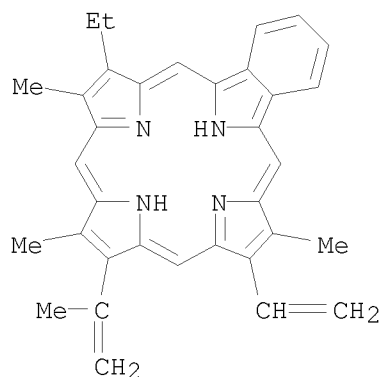
L9 ANSWER 85 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1991:471237 CAPLUS  
 DOCUMENT NUMBER: 115:71237  
 ORIGINAL REFERENCE NO.: 115:12303a,12306a  
 TITLE: Total synthesis of chlorophyll c fossils and related  
 petroporphyrins  
 AUTHOR(S): Bauder, Claude; Ocampo, Ruben; Callot, Henry J.  
 CORPORATE SOURCE: Inst. Chim., Univ. Louis Pasteur, Strasbourg, 67000,  
 Fr.  
 SOURCE: Tetrahedron Letters (1991), 32(22), 2537-40  
 CODEN: TELEAY; ISSN: 0040-4039  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



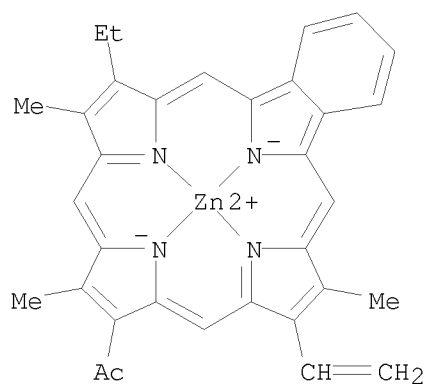
AB Petroporphyrins I [R = Me, R1 = Et; RR1 = (CH2)4] and II, related to  
 chlorophyll c were prepared via cyclization of an isopropenyl group.  
 IT 135241-24-6  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (complexation and acetylation of)  
 RN 135241-24-6 CAPLUS  
 CN 23H,25H-Benzo[b]porphine, 18-(2-chloroethyl)-8-ethyl-9,13,19-trimethyl-  
 (9CI) (CA INDEX NAME)



IT 135241-30-4P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (preparation and cyclization of)  
 RN 135241-30-4 CAPLUS  
 CN 23H,25H-Benzo[b]porphine, 9-ethenyl-19-ethyl-8,14,18-trimethyl-13-(1-  
 methylethenyl)- (9CI) (CA INDEX NAME)

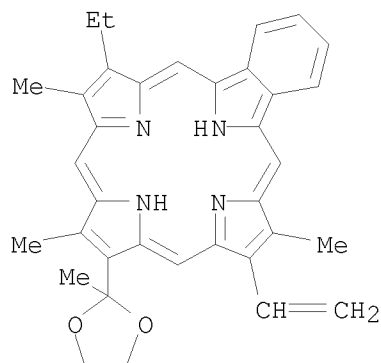


IT 135162-66-2P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (preparation and methylenation of)  
 RN 135162-66-2 CAPLUS  
 CN Zinc, [1-(9-ethenyl-19-ethyl-8,14,18-trimethyl-23H,25H-benzo[b]porphin-13-yl)ethanonato(2-)-N23,N24,N25,N26]-, (SP-4-2)- (9CI) (CA INDEX NAME)

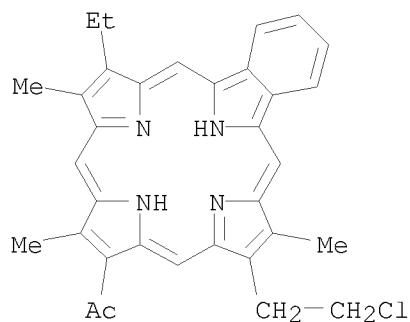


IT 135241-28-0P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation, acetal hydrolysis, and complexation of)  
 RN 135241-28-0 CAPLUS  
 CN 23H,25H-Benzo[b]porphine, 9-ethenyl-19-ethyl-8,14,18-trimethyl-13-(2-methyl-1,3-dioxolan-2-yl)- (9CI) (CA INDEX NAME)





IT 135241-26-8P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (preparation, ketalization, and dehydrochlorination of)  
 RN 135241-26-8 CAPLUS  
 CN Ethanone, 1-[9-(2-chloroethyl)-19-ethyl-8,14,18-trimethyl-23H,25H-  
 benzo[b]porphin-13-yl]- (9CI) (CA INDEX NAME)



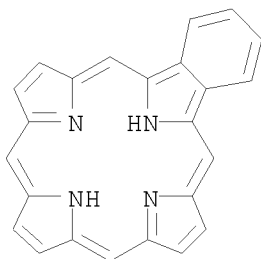
L9 ANSWER 86 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1991:17561 CAPLUS  
 DOCUMENT NUMBER: 114:17561  
 ORIGINAL REFERENCE NO.: 114:2997a,3000a  
 TITLE: Pre-activated therapeutic agents derived from  
 photoactive compounds  
 INVENTOR(S): Gulliya, Kirpal S.; Pervaiz, Shazib; Matthews, J.  
 Lester; Dowben, Robert M.; Newman, Joseph T.; Forest,  
 Edward  
 PATENT ASSIGNEE(S): Baylor Research Foundation, USA  
 SOURCE: PCT Int. Appl., 62 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
------------	------	------	-----------------	------

```

-----
WO 9003187      A1      19900405      WO 1989-US4181      19890926
W: AU, DK, FI, HU, JP, NO, SU
RW: AT, BE, CH, DE, FR, GB, IT, NL, SE
US 5091385      A      19920225      US 1988-252256      19880930
AU 8943450      A      19900418      AU 1989-43450      19890926
AU 631142      B2      19921119
EP 436642      A1      19910717      EP 1989-911468      19890926
EP 436642      B1      19950426
R: AT, BE, CH, DE, FR, GB, IT, LI, NL, SE
JP 04501717      T      19920326      JP 1989-510674      19890926
JP 2807682      B2      19981008
CA 1329120      C      19940503      CA 1989-613203      19890926
AT 121630      T      19950515      AT 1989-911468      19890926
US 5177073      A      19930105      US 1990-509036      19900413
US 5489590      A      19960206      US 1992-829933      19920203
PRIORITY APPLN. INFO.:      US 1988-252256      A 19880930
                                WO 1989-US4181      A 19890926
                                US 1990-509036      A3 19900413
AB  Photoactive neoplasm inhibitors, such as Merocyanine 540,
    dihematoporphyrin ether, porphyrin, benzoporphyrin, etc., are preactivated
    with radiation, electromagnetic or elec. energy, prior to use.
    Laser-activated Merocyanine 540 (40 µg/mL) was toxic to HL-60 human
    leukemia and L1210 murine leukemia cells, in vitro, without affecting
    human blood lymphocytes.
IT  36469-17-7, 23H,25H-Benzo[b]porphine
    RL: BAC (Biological activity or effector, except adverse); BSU (Biological
    study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES
    (Uses)
        (neoplasm inhibitor, photoactive, preactivation of)
RN  36469-17-7  CAPLUS
CN  23H,25H-Benzo[b]porphine (9CI)  (CA INDEX NAME)

```



```

L9  ANSWER 87 OF 103  CAPLUS  COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER:      1990:500475  CAPLUS
DOCUMENT NUMBER:       113:100475
ORIGINAL REFERENCE NO.: 113:16959a,16962a
TITLE:
    Preliminary characterization of porphyrins from the
    Gafsa Basin, Tunisia: evidence for metal-free benzo
    porphyrins from an immature sediment
AUTHOR(S):
    Quirke, J. Martin E.; Dale, T.; Britton, Edward D.;
    Yost, Richard A.; Trichet, Jean; Belayouni, H.
CORPORATE SOURCE:
    Dep. Chem., Florida Int. Univ., Miami, FL, 33199, USA
SOURCE:
    Organic Geochemistry (1990), 15(2), 169-77

```

CODEN: ORGEDE; ISSN: 0146-6380

DOCUMENT TYPE: Journal

LANGUAGE: English

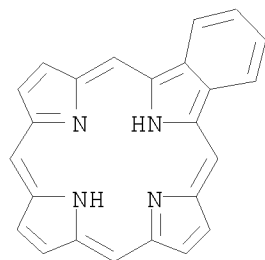
AB Five metal-free porphyrin fractions were isolated chromatog. from an immature chert of the Gafsa Basin (Paleocene, Tunisia). Each fraction was analyzed by electron ionization tandem mass spectrometry. In addition to the expected aetioporphyrin-III and deoxophylloerythroetioporphyrin (DPEP), an isomeric C32 CAP porphyrin, which probably bears an extended isocyclic ring, was also detected. A C31 CAP component bearing one unsubstituted  $\beta$ -position was isolated. C33 and C34 benzo-DPEP porphyrin as well as a C33 tetrahydrobenzo-DPEP porphyrin were also present, which indicates that such compds. are generated in immature sediments.

IT 36469-17-7, 23H,25H-Benzo[b]porphine 128920-36-5

RL: GOC (Geological or astronomical occurrence); OCCU (Occurrence)  
(in immature chert, of Gafsa Basin, Tunisia)

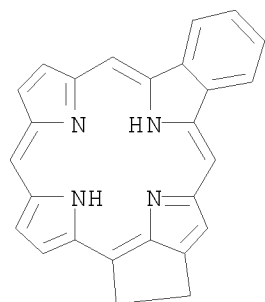
RN 36469-17-7 CAPLUS

CN 23H,25H-Benzo[b]porphine (9CI) (CA INDEX NAME)



RN 128920-36-5 CAPLUS

CN 5,22:12,15-Diimino-20,18-metheno-7,10-nitrilobenzo[o]cyclopent[b]azacyclononadecine, 16,17-dihydro- (9CI) (CA INDEX NAME)



L9 ANSWER 88 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1990:406010 CAPLUS

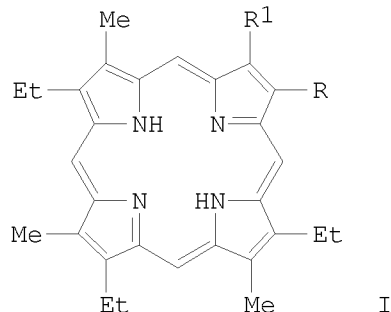
DOCUMENT NUMBER: 113:6010

ORIGINAL REFERENCE NO.: 113:1163a,1166a

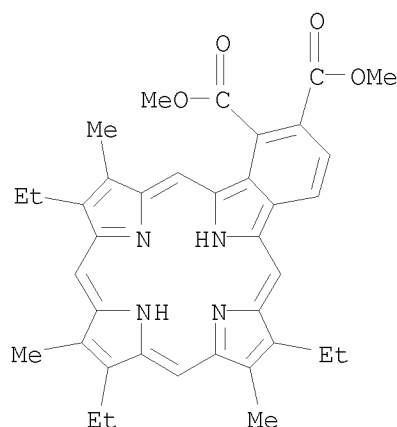
TITLE: Transformation of a monovinylporphyrin to  
benzoporphyrins via Diels-Alder adducts

AUTHOR(S): Yon-Hin, Paul; Wijesekera, Tilak P.; Dolphin, David

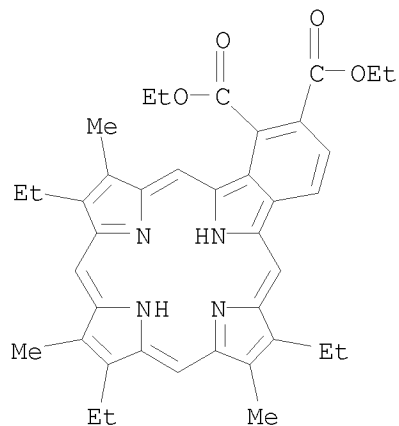
CORPORATE SOURCE: Dep. Chem., Univ. British Columbia, Vancouver, BC, V6T 1Y6, Can.  
 SOURCE: Tetrahedron Letters (1989), 30(45), 6135-8  
 CODEN: TELEAY; ISSN: 0040-4039  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 113:6010  
 GI



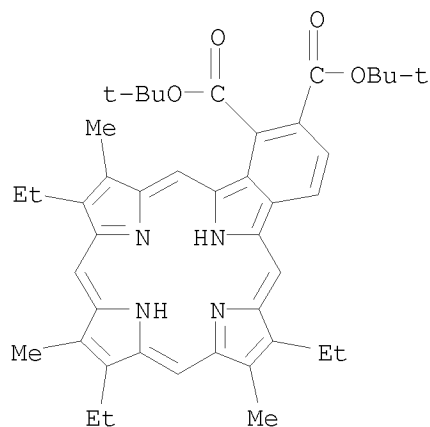
AB Vinylporphyrin I ( $R = \text{CH}:\text{CH}_2$ ,  $R_1 = \text{H}$ ) has been synthesized and treated with excess  $\text{R}_2\text{CC}(\text{t})\text{CO}_2\text{R}$  ( $R = \text{Me, Et, CMe}_3$ ) to give monobenzoporphyrins I [ $\text{RR}_1 = \text{CH}:\text{CHC}(\text{CO}_2\text{R})\text{:C}(\text{CO}_2\text{R})$ ] in high yield. Evidence suggests that the initial adduct isomerizes to a new porphyrin [I,  $\text{RR}_1 = \text{CH}_2\text{CH}_2\text{C}(\text{CO}_2\text{R})\text{:C}(\text{CO}_2\text{R})$ ] en route to the benzoporphyrin.  
 IT 127640-31-7P 127640-32-8P 127640-33-9P  
 RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)  
 RN 127640-31-7 CAPLUS  
 CN 23H,25H-Benzo[b]porphine-1,2-dicarboxylic acid, 8,13,18-triethyl-9,14,19-trimethyl-, dimethyl ester (9CI) (CA INDEX NAME)



RN 127640-32-8 CAPLUS  
 CN 23H,25H-Benzo[b]porphine-1,2-dicarboxylic acid, 8,13,18-triethyl-9,14,19-trimethyl-, diethyl ester (9CI) (CA INDEX NAME)



RN 127640-33-9 CAPLUS  
 CN 23H,25H-Benzo[b]porphine-1,2-dicarboxylic acid,  
 8,13,18-triethyl-9,14,19-trimethyl-, bis(1,1-dimethylethyl) ester (9CI)  
 (CA INDEX NAME)



L9 ANSWER 89 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1989:577632 CAPLUS  
 DOCUMENT NUMBER: 111:177632  
 ORIGINAL REFERENCE NO.: 111:29547a,29550a  
 TITLE: The Henryville Bed of the New Albany shale - I.  
 Preliminary characterization of the nickel and vanadyl  
 porphyrins in the bitumen  
 AUTHOR(S): Van Berkel, Gary J.; Quirke, J. Martin E.; Filby,  
 Royston H.  
 CORPORATE SOURCE: Dep. Chem., Washington State Univ., Pullman, WA,  
 99164-1300, USA  
 SOURCE: Organic Geochemistry (1989), 14(2), 119-28  
 CODEN: ORGEDE; ISSN: 0146-6380  
 DOCUMENT TYPE: Journal

LANGUAGE: English

AB The Ni, V, Ni(II) porphyrin and VO(II) porphyrin concns. in the bitumen of an organic rich sample of the Henryville Bed of the New Albany shale (Mississippian-Devonian; Indiana, U.S.A.) were determined. The bitumen contains 1776  $\mu\text{g}$  Ni/g and 1550  $\mu\text{g}$  V/g bitumen. The porphyrin concns. of 9900  $\mu\text{g}$ /g and 9100  $\mu\text{g}$ /g, resp., are higher than those reported in most source rock bitumens or crude oils. The similar abundances of Ni(II) and VO(II) porphyrins indicates a depositional environment being transitional between strongly anoxic (VO(II) porphyrins dominant) and less anoxic in which Ni(II) porphyrins dominate. The Ni(II) and VO(II) porphyrins in the bitumen occur as etioporphyrin (I), deoxophylloerythroetioporphyrin (DPEP), and tetrahydrobenzo-DPEP (THBD) species in the order of abundance: I > DPEP > THBD for Ni(II) and DPEP > I > THBD for VO(II) porphyrins. The DPEP/etio ratios of 1.4 for the VO(II) series and 0.91 for the Ni(II) series and a vitrinite reflectance of 0.5-0.6% are consistent with the organic matter in the New Albany shale being of intermediate maturity. The C-number distributions of the I, DPEP, and THBD porphyrins of the 2 metals are very similar. This similarity and the fact that C nos. of both Ni(II) and VO(II) porphyrins extend at least to C36 suggests that the Ni(II) and VO(II) porphyrins originated via similar geochem. pathways in the New Albany shale. The major pathway was the porphyrins release during kerogen catagenesis.

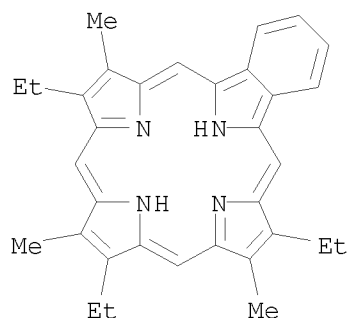
IT 93614-17-6

RL: USES (Uses)

(in bitumen, of New Albany, Indiana)

RN 93614-17-6 CAPLUS

CN 23H,25H-Benzo[b]porphine, 8,13,18-triethyl-9,14,19-trimethyl- (9CI) (CA INDEX NAME)



L9 ANSWER 90 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1989:453350 CAPLUS

DOCUMENT NUMBER: 111:53350

ORIGINAL REFERENCE NO.: 111:8997a,9000a

TITLE: In vitro photosensitization with a benzoporphyrin derivative

AUTHOR(S): Kessel, David

CORPORATE SOURCE: Sch. Med., Wayne State Univ., Detroit, MI, 48201, USA

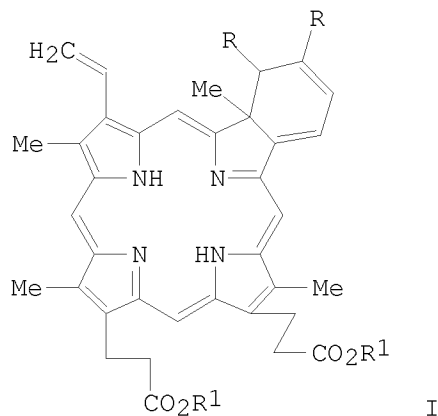
SOURCE: Photochemistry and Photobiology (1989), 49(5), 579-82

CODEN: PHCBAP; ISSN: 0031-8655

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



AB Biophys. and photobiol. properties of 2 benzoporphyrin derivs., (I, R = COOEt, R'=H or Me) were examined These dyes exhibit substantial absorbance in the red, and are potent photosensitizers in L1210 cells. After brief (0.5 h) incubations, phototoxicity was more closely correlated with membrane than with mitochondrial photodamage. Affinity of these dyes toward plasma lipoproteins are consistent with a mode of localization via the low-d. lipoprotein-mediated mechanism utilized by HPD.

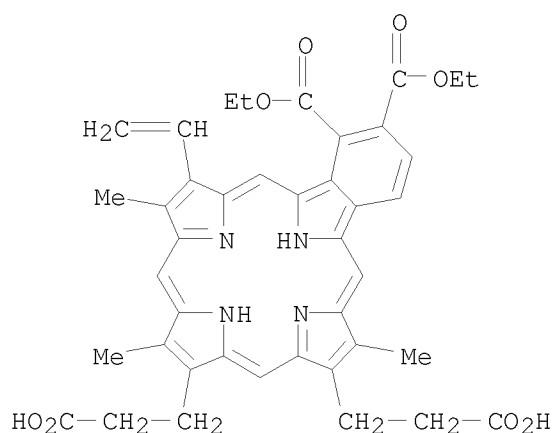
IT 121714-54-3

RL: BIOL (Biological study)

(photosensitization by, of mammalian cells with visible light, photophys. properties in relation to)

RN 121714-54-3 CAPLUS

CN 23H,25H-Benzo[b]porphine-9,13-dipropanoic acid, 1,2-bis(ethoxycarbonyl)-19-ethenyl-8,14,18-trimethyl- (9CI) (CA INDEX NAME)



L9 ANSWER 91 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 1987:601590 CAPLUS

10583126.trn

DOCUMENT NUMBER: 107:201590  
 ORIGINAL REFERENCE NO.: 107:32323a,32326a  
 TITLE: Vanadylporphyrins in crude oil of Russian field  
 AUTHOR(S): Zabarova, D. Z.; Serebrennikova, O. V.  
 CORPORATE SOURCE: Inst. Khim. Nefti, Tomsk, USSR  
 SOURCE: Neftekhimiya (1987), 27(4), 435-8  
 CODEN: NEFTAH; ISSN: 0028-2421  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Russian

AB Petroleum of the Russkoe field contains 0.014  $\mu\text{mol/g}$  VO porphyrins. In the vacuum distillation of this petroleum 12% of these porphyrins pass to the distillates. The variety of porphyrin structures in the bottoms is larger than in the petroleum.

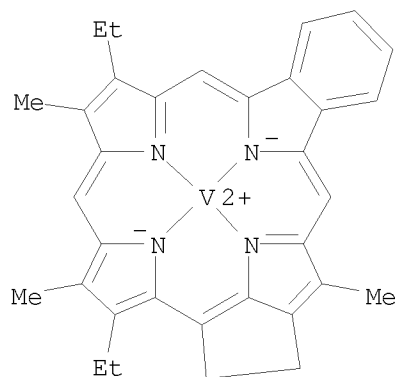
IT 111256-74-7

RL: USES (Uses)

(in petroleum, fate of, in vacuum distillation)

RN 111256-74-7 CAPLUS

CN Vanadium, [8,14-diethyl-16,17-dihydro-9,13,24-trimethyl-5,22:12,15-diimino-20,18-metheno-7,10-nitrilobenzo[o]cyclopent[b]azacyclononadecinato(2-)-N19,N23,N25,N26]-, (SP-4-2)- (9CI) (CA INDEX NAME)



L9 ANSWER 92 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1987:52812 CAPLUS

DOCUMENT NUMBER: 106:52812

ORIGINAL REFERENCE NO.: 106:8715a,8718a

TITLE: Comparative computerized gas chromatographic-mass spectrometric analysis of petroporphyrins

AUTHOR(S): Gill, J. P.; Evershed, R. P.; Eglinton, G.

CORPORATE SOURCE: Sch. Chem., Univ. Bristol, Bristol, BS8 1TS, UK

SOURCE: Journal of Chromatography (1986), 369(2), 281-312

CODEN: JOCRAM; ISSN: 0021-9673

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The ability of computerized gas chromatog.-mass spectrometry (C-GC-MS) to afford detailed information on petroporphyrin composition is exemplified through analyses of Boscan crude oil and La Luna shale (Maracaibo Basin, Venezuela), an oil-source rock pair. The petroporphyrins of both samples are complex mixts., comprising at least 224 and 175 compds., resp. Five structural classes already characterized, showed at least 5 pseudo-homologous series through linear Kovats' plots and co-injection.



The 2 samples are qual. and quant. very similar in composition. These related samples are compared and contrasted with an unrelated bitumen, gilsonite, examined in an earlier paper. The data showed that petroporphyrin anal. by C-GC-MS can provide classical biol. marker information, e.g. thermal maturity. This paper provides the first such comparative examination of petroporphyrins by GC-MS anal.

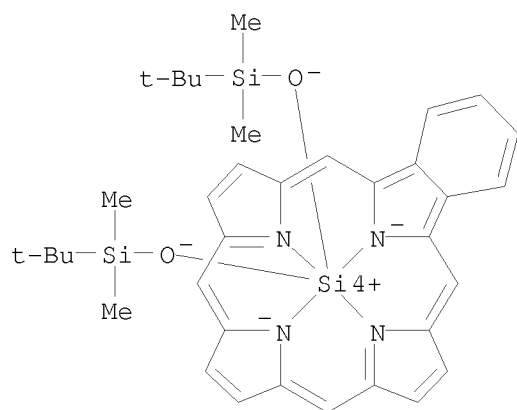
IT 106374-69-0D, alkyl derivs. 106397-85-7D, alkyl derivs.

RL: ANT (Analyte); ANST (Analytical study)

(determination of, in anal. of petroleum and shale, by computerized gas chromatog.-mass spectrometry, of Maracaibo Basin, Venezuela)

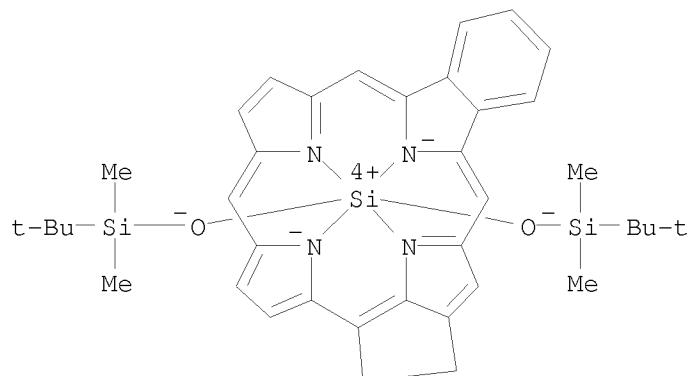
RN 106374-69-0 CAPLUS

CN Silicon, bis[(1,1-dimethylethyl)dimethylsilanolato][23H,25H-benzo[b]porphinato(2-)-N23,N24,N25,N26]-, (OC-6-12)- (9CI) (CA INDEX NAME)



RN 106397-85-7 CAPLUS

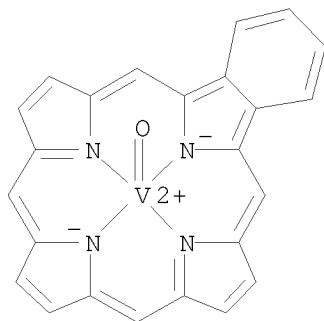
CN Silicon, [16,17-dihydro-5,22:12,15-diimino-20,18-metheno-7,10-nitrilobenzo[o]cyclopent[b]azacyclononadecinato(2-)-N19,N23,N25,N26]bis[(1,1-dimethylethyl)dimethylsilanolato]-, (OC-6-13)- (9CI) (CA INDEX NAME)



L9 ANSWER 93 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 1986:431769 CAPLUS

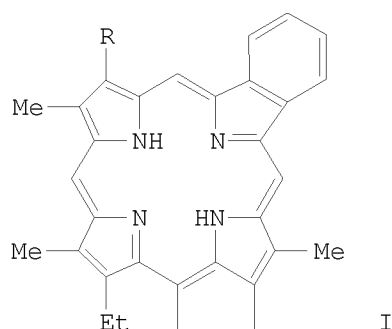
10583126.trn

DOCUMENT NUMBER: 105:31769  
 ORIGINAL REFERENCE NO.: 105:5161a, 5164a  
 TITLE: Oxygen electroreduction on porphyrins derived from petroleum  
 AUTHOR(S): Radyushkina, K. A.; Tarasevich, M. R.; Novikova, E. M.; Kublanovskii, V. S.; Antipenko, V. R.; Zemtseva, L. I.  
 CORPORATE SOURCE: Inst. Elektrokhim. im. Frumkina, Moscow, USSR  
 SOURCE: Doklady Akademii Nauk SSSR (1986), 288(2), 397-400 [Chem.]  
 CODEN: DANKAS; ISSN: 0002-3264  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Russian  
 AB The use of natural porphyrins as raw materials for pyrolysis to obtain catalysts for O electroredn. is considered. The pyrolysis of petroleum porphyrins deposited from raw materials can be used to obtain such catalysts which have as good or better activity than does the pyrolyzed synthetic material Co tetra(p-methoxyphenyl)-porphyrin. The electrocatalytic activity of petroleum-derived porphyrins was evaluated by measuring the steady-state polarization curves of the electroredn. of O in 1M KOH and 0.5M H2SO4 on floating gas-diffusion electrodes.  
 IT 99625-79-3  
 RL: CAT (Catalyst use); USES (Uses)  
 (catalysts, for electroredn. of oxygen)  
 RN 99625-79-3 CAPLUS  
 CN Vanadium, [23H,25H-benzo[b]porphinato(2-)-N23,N24,N25,N26]oxo-, (SP-5-12)-(9CI) (CA INDEX NAME)



L9 ANSWER 94 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1986:148606 CAPLUS  
 DOCUMENT NUMBER: 104:148606  
 ORIGINAL REFERENCE NO.: 104:23513a, 23516a  
 TITLE: Naturally occurring benzoporphyrins: bacterial marker pigments?  
 AUTHOR(S): Kaur, Surinder; Chicarelli, M. Ines; Maxwell, James R.  
 CORPORATE SOURCE: Sch. Chem., Univ. Bristol, Bristol, BS8 1TS, UK  
 SOURCE: Journal of the American Chemical Society (1986), 108(6), 1347-8  
 CODEN: JACSAT; ISSN: 0002-7863  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 104:148606

GI



AB A C33 and a C32 monobenzo[g]porphyrin with an exocyclic ethano ring (I, R = Et, Me), each present in Boscan crude oil (Cretaceous, Venezuela) as the vanadyl complex, have been isolated as the demetalated species. Their structures have been determined by  $^1\text{H}$  NMR spectroscopic anal. of the  $\text{ZnII}$  complexes, using decoupling and nuclear Overhauser effect expts. The origin of these compds. is unclear, but it is possible that they may have arisen from precursors related to bacteriochlorophylls-d.

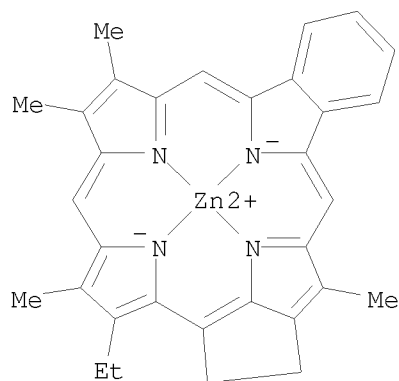
IT 100813-33-0

RL: PRP (Properties)

(NMR of)

RN 100813-33-0 CAPLUS

CN Zinc, [14-ethyl-16,17-dihydro-8,9,13,24-tetramethyl-5,22:12,15-diimino-20,18-metheno-7,10-nitrilobenzo[o]cyclopent[b]azacyclononadecinato(2-)- $\kappa\text{N}19,\kappa\text{N}23,\kappa\text{N}25,\kappa\text{N}26$ ]-, (SP-4-2)- (9CI) (CA INDEX NAME)



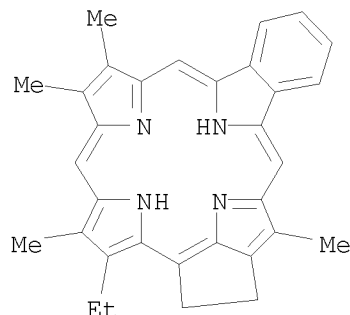
IT 100813-32-9P

RL: PREP (Preparation)

(isolation of, from petroleum, and mol. structure of)

RN 100813-32-9 CAPLUS

CN 5,22:12,15-Diimino-20,18-metheno-7,10-nitrilobenzo[o]cyclopent[b]azacyclononadecine, 14-ethyl-16,17-dihydro-8,9,13,24-tetramethyl- (9CI) (CA INDEX NAME)



L9 ANSWER 95 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1986:26086 CAPLUS

DOCUMENT NUMBER: 104:26086

ORIGINAL REFERENCE NO.: 104:4197a,4200a

TITLE: Petroleum porphyrins-electrocatalysts for cathodic oxygen reduction

AUTHOR(S): Radyushkina, K. A.; Antipenko, V. R.; Novikova, E. M.; Pevneva, G. S.; Tarasevich, M. R.; Kublanovskii, V. S.

CORPORATE SOURCE: Inst. Elektrokhim. im. Frumkina, Moscow, USSR

SOURCE: Elektrokhimiya (1985), 21(10), 1390-3

CODEN: ELKKAX; ISSN: 0424-8570

DOCUMENT TYPE: Journal

LANGUAGE: Russian

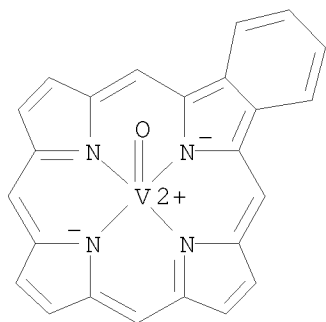
AB The possibility was studied of obtaining active catalysts for the cathodic reduction of O by pyrolysis on C of concs. of vanadyl porphyrins, deposited from crude petroleum expts. by DMF with subsequent chromatog. purification of the extract on Al<sub>2</sub>O<sub>3</sub> and silica gel. The electrochem. measurements were carried out on floating gas-diffusion electrodes made from wetproofed C black on which a very thin layer ( $\leq 1$  mg/cm<sup>2</sup>) of catalyst is deposited. Polarization curves were plotted of the reduction of O in of 1N KOH and 1N H<sub>2</sub>SO<sub>4</sub> at 20° on the initial vanadylporphyrins, the products of their pyrolysis in a He atmospheric at 800° (30 min), the products of pyrolysis of a mixture of vanadyl porphyrins (10 weight%) and modified active C. The prospects of using natural vanadyl porphyrins for electrocatalysis of O reactions in an alkaline medium are good.

IT 99625-79-3D, derivs.

RL: PRP (Properties)  
(electrocatalyst, for oxygen reduction)

RN 99625-79-3 CAPLUS

CN Vanadium, [23H,25H-benzo[b]porphinato(2-)-N23,N24,N25,N26]oxo-, (SP-5-12)-(9CI) (CA INDEX NAME)



L9 ANSWER 96 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1985:72048 CAPLUS

DOCUMENT NUMBER: 102:72048

ORIGINAL REFERENCE NO.: 102:11165a,11168a

TITLE: Computerized gas chromatographic-mass spectrometric analysis of complex mixtures of alkyl porphyrins

AUTHOR(S): Marriott, P. J.; Gill, J. P.; Evershed, R. P.; Hein, C. S.; Eglinton, G.

CORPORATE SOURCE: Sch. Chem., Univ. Bristol, Bristol, BS8 1TS, UK

SOURCE: Journal of Chromatography (1984), 301(1), 107-28

CODEN: JOCRAM; ISSN: 0021-9673

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Computerized capillary gas chromatog.-mass spectrometry (GC-MS) anal. of complex mixts. of alkyl porphyrins, as their bis(trimethylsiloxy)silicon(IV) and bis(tert-butyldimethylsiloxy)silicon(IV) derivs., is described. The latter derivative is more suitable for routine GC-MS anal. This computerized GC-MS approach, when applied to the alkyl porphyrins of 2 geol. samples, a bitumen (Gilsonite, Eocene age, UT, U.S.A.) and a crude oil (Boscan, Cretaceous age, West Venezuela), has revealed the highly complex compns. of these fractions. Computer-aided data processing, using relative retention index calcns., facilitated the classification of the chromatog. peaks according to structural type and membership of pseudo-homologous series. Computerized GC-MS is compared with, and contrasted to high-performance liquid chromatog. as a means of petroporphyrin anal.

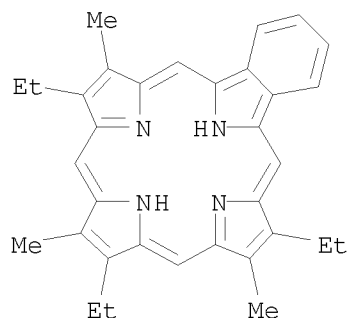
IT 93614-17-6D, bis(tert-butyldimethylsiloxy)silicon derivs.

93614-18-7D, bis(tert-butyldimethylsiloxy)silicon derivs.

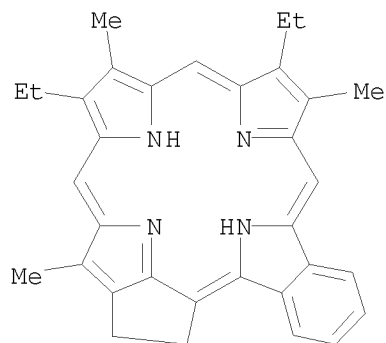
RL: PRP (Properties); ANST (Analytical study)  
(mass spectra of)

RN 93614-17-6 CAPLUS

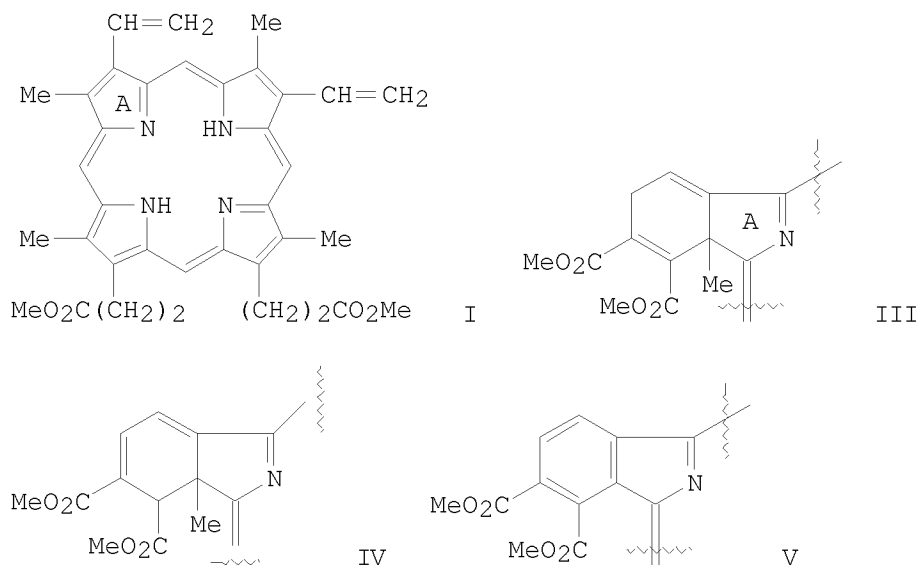
CN 23H,25H-Benzo[b]porphine, 8,13,18-triethyl-9,14,19-trimethyl- (9CI) (CA INDEX NAME)



RN 93614-18-7 CAPLUS  
 CN 7,10:17,22-Diimino-5,3-metheno-12,15-nitrilobenzo[e]cyclopent[b]azacyclononadecine, 8,13-diethyl-1,2-dihydro-9,14,26-trimethyl- (9CI) (CA INDEX NAME)



L9 ANSWER 97 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1985:61981 CAPLUS  
 DOCUMENT NUMBER: 102:61981  
 ORIGINAL REFERENCE NO.: 102:9713a,9716a  
 TITLE: Ready syntheses of benzoporphyrins via Diels-Alder reactions with protoporphyrin IX  
 AUTHOR(S): Morgan, Alan R.; Pangka, Veronica Scherrer; Dolphin, David  
 CORPORATE SOURCE: Dep. Chem., Univ. British Columbia, Vancouver, V6T 1Y6, Can.  
 SOURCE: Journal of the Chemical Society, Chemical Communications (1984), (16), 1047-8  
 CODEN: JCCCAT; ISSN: 0022-4936  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



AB Protoporphyrin IX di-Me ester (I) underwent Diels-Alder reaction with strongly activated dienophiles; the resulting adducts underwent elimination of the angular Me group to give monobenzoporphyrins. E.g., reaction of I with  $\text{MeO}_2\text{C} \cdot \text{C} \equiv \text{C} \cdot \text{CO}_2\text{Me}$  (II) gave the adduct III, which rearranged to IV on treatment with  $\text{Et}_3\text{N}$ . IV aromatized on treatment with excess II and  $\text{Et}_3\text{N}$  to give the benzoporphyrin V.

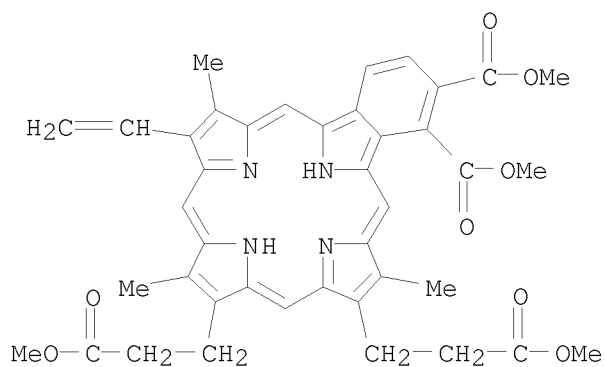
IT 94238-26-3P 94238-28-5P 94238-34-3P

94238-36-5P 94238-37-6P 94238-42-3P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 94238-26-3 CAPLUS

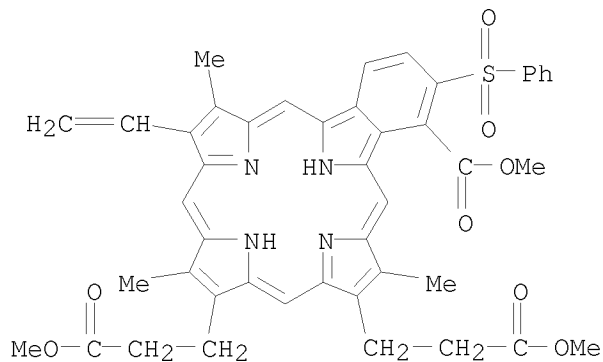
CN 23H,25H-Benzo[b]porphine-9,13-dipropanoic acid,  
18-ethenyl-3,4-bis(methoxycarbonyl)-8,14,19-trimethyl-, dimethyl ester  
(9CI) (CA INDEX NAME)



RN 94238-28-5 CAPLUS

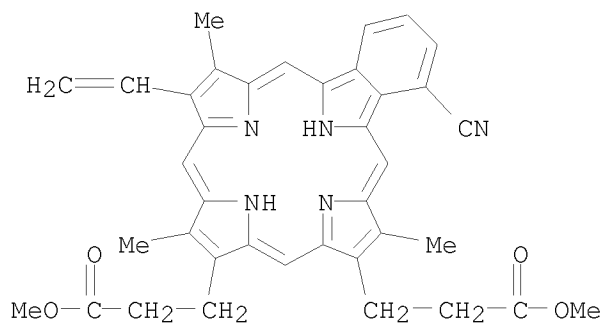
CN 23H,25H-Benzo[b]porphine-9,13-dipropanoic acid,

18-ethenyl-4-(methoxycarbonyl)-8,14,19-trimethyl-3-(phenylsulfonyl)-,  
dimethyl ester (9CI) (CA INDEX NAME)



RN 94238-34-3 CAPLUS

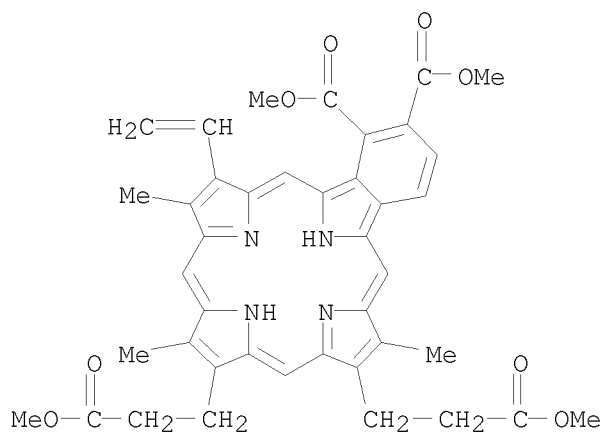
CN 23H,25H-Benzo[b]porphine-9,13-dipropanoic acid,  
4-cyano-18-ethenyl-8,14,19-trimethyl-, dimethyl ester (9CI) (CA INDEX  
NAME)



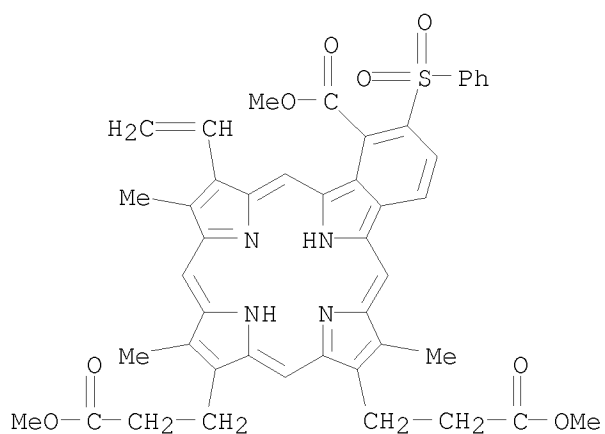
RN 94238-36-5 CAPLUS

CN 23H,25H-Benzo[b]porphine-9,13-dipropanoic acid,  
19-ethenyl-1,2-bis(methoxycarbonyl)-8,14,18-trimethyl-, dimethyl ester  
(9CI) (CA INDEX NAME)

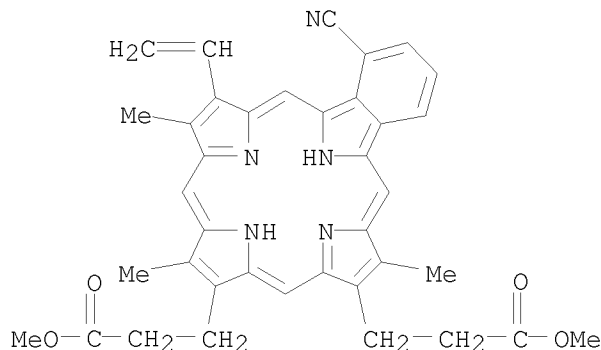




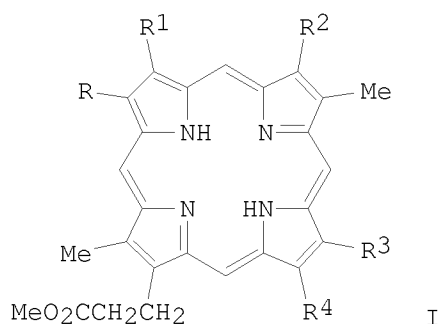
RN 94238-37-6 CAPLUS  
 CN 23H,25H-Benzo[b]porphine-9,13-dipropanoic acid,  
 19-ethenyl-1-(methoxycarbonyl)-8,14,18-trimethyl-2-(phenylsulfonyl)-,  
 dimethyl ester (9CI) (CA INDEX NAME)



RN 94238-42-3 CAPLUS  
 CN 23H,25H-Benzo[b]porphine-9,13-dipropanoic acid,  
 1-cyano-19-ethenyl-8,14,18-trimethyl-, dimethyl ester (9CI) (CA INDEX  
 NAME)

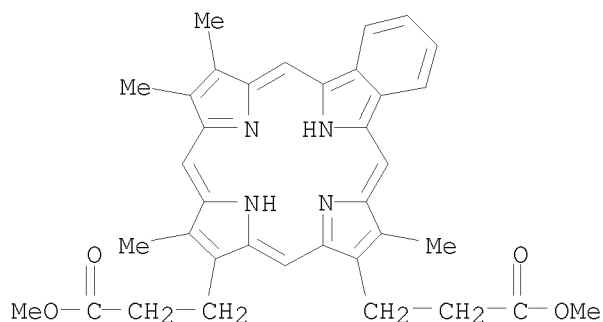


L9 ANSWER 98 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1983:34416 CAPLUS  
 DOCUMENT NUMBER: 98:34416  
 ORIGINAL REFERENCE NO.: 98:5381a,5384a  
 TITLE: Chemistry of pyrrolic compounds. LI. Porphyrins with  
 electron-withdrawing groups in the same pyrrolic ring:  
 preparation of a pyridazinoporphyrin  
 AUTHOR(S): Chaudhry, Irshad A.; Clezy, Peter S.  
 CORPORATE SOURCE: Dep. Org. Chem., Univ. New South Wales, Kensington,  
 2033, Australia  
 SOURCE: Australian Journal of Chemistry (1982), 35(6),  
 1185-201  
 CODEN: AJCHAS; ISSN: 0004-9425  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI

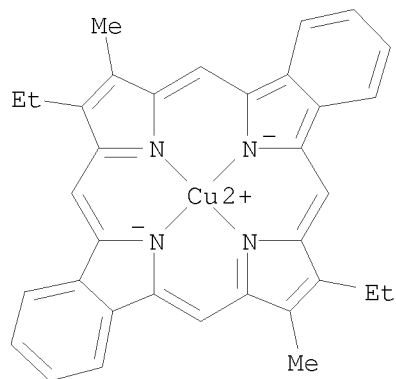


AB Porphyrins I (R = R1 = CH2CH2OH, CH2CH2Cl, CH:CH2, CHO, R2 = R3 = Me, R4 =  
 CH2CH2CO2Me; R = CHO, R1 = CO2Me, R = CO2Me, R1 = CHO, R2 = R3 = Me, R4 =  
 CH2CH2CO2Me; R = R1 = R3 = R4 = CH2CH2OHc, CH2CH2Cl, CH:CH2, R2 =  
 CH2CH2CO2Me) were prepared by known methods. Oxidation of I (R = R1 = CH:CH2,  
 R2 = R3 = Me, R4 = CH2CH2CO2Me) gave I (RR1 = CH:CHCH:CH, R2 = R3 = Me, R4  
 = CH2CH2CO2Me). I (RR1 = CH:NN:CH, R2 = R3 = Me, R4 = CH2CH2CO2Me) was  
 obtained by treating I (R = R1 = CHO, R1 = R2 = Me, R4 = CH2CH2CO2Me) with  
 N2H4.  
 IT 84089-93-0P

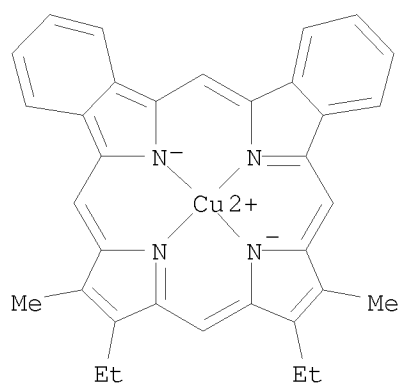
RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 RN 84089-93-0 CAPLUS  
 CN 23H,25H-Benzo[b]porphine-9,13-dipropanoic acid, 8,14,18,19-tetramethyl-,  
 dimethyl ester (9CI) (CA INDEX NAME)



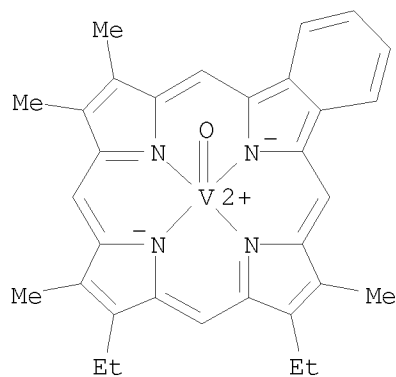
L9 ANSWER 99 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1982:406035 CAPLUS  
 DOCUMENT NUMBER: 97:6035  
 ORIGINAL REFERENCE NO.: 97:1163a,1166a  
 TITLE: The chemistry of pyrrolic compounds. XLIX. Further  
 observations on the chemistry of the benzoporphyrins  
 AUTHOR(S): Clezy, Peter S.; Mirza, Aminul H.  
 CORPORATE SOURCE: Dep. Org. Chem., Univ. New South Wales, Kensington,  
 2033, Australia  
 SOURCE: Australian Journal of Chemistry (1982), 35(1), 197-209  
 CODEN: AJCHAS; ISSN: 0004-9425  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Isomeric dibenzoporphyrins having the fused rings attached to either  
 adjacent or opposite pyrrolic rings have been prepared and their properties  
 compared. The chemical of some of the intermediates encountered during the  
 synthesis of a benzoporphyrin has been examined  
 IT 81923-08-2P 81923-09-3P 81966-00-9P  
 81976-21-8P 81976-22-9P 81976-23-0P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 RN 81923-08-2 CAPLUS  
 CN Copper, [8,20-diethyl-9,21-dimethyl-25H,27H-dibenzo[b,l]porphinato(2-)-  
 N25,N26,N27,N28]-, (SP-4-1)- (9CI) (CA INDEX NAME)



RN 81923-09-3 CAPLUS  
 CN Copper, [9,12-diethyl-8,13-dimethyl-25H,27H-dibenzo[b,g]porphinato(2-)-N25,N26,N27,N28]-, (SP-4-2)- (9CI) (CA INDEX NAME)

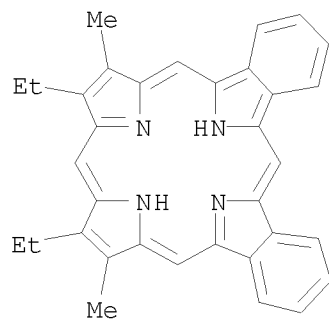


RN 81966-00-9 CAPLUS  
 CN Vanadium, [9,13-diethyl-8,14,18,19-tetramethyl-23H,25H-benzo[b]porphinato(2-)-N23,N24,N25,N26]oxo-, (SP-5-13)- (9CI) (CA INDEX NAME)



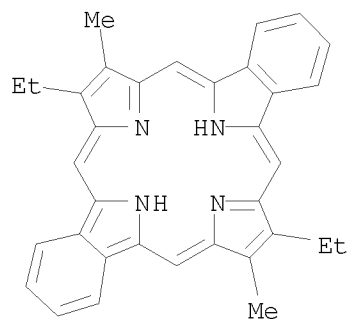
RN 81976-21-8 CAPLUS

CN 25H,27H-Dibenzo[b,g]porphine, 9,13-diethyl-8,14-dimethyl- (9CI) (CA INDEX NAME)



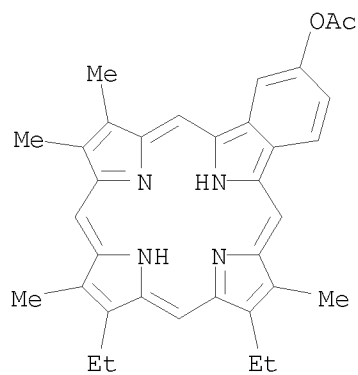
RN 81976-22-9 CAPLUS

CN 25H,27H-Dibenzo[b,l]porphine, 8,20-diethyl-9,21-dimethyl- (9CI) (CA INDEX NAME)



RN 81976-23-0 CAPLUS

CN 23H,25H-Benzo[b]porphin-2-ol, 9,13-diethyl-8,14,18,19-tetramethyl-, acetate (ester) (9CI) (CA INDEX NAME)



L9 ANSWER 100 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1982:34078 CAPLUS

DOCUMENT NUMBER: 96:34078

ORIGINAL REFERENCE NO.: 96:5629a,5632a

TITLE: MO LCAO SCF method for the calculation of magnetic characteristics of porphyrin molecules

AUTHOR(S): Vysotskii, Yu. B.; Kuz'mitskii, V. A.; Solov'ev, K. N.

CORPORATE SOURCE: Inst. Fiz.-Org. Khim. Uglekhim., Kiev, USSR

SOURCE: Zhurnal Strukturnoi Khimii (1981), 22(4), 22-30

CODEN: ZSTKAI; ISSN: 0044-4634

DOCUMENT TYPE: Journal

LANGUAGE: Russian

AB The <sup>1</sup>H, <sup>13</sup>C and <sup>15</sup>N NMR chemical shifts of several porphyrins were calculated from the ring currents and charge distributions, obtained by PMO calcns. with the London approximation The  $\pi$ -electron ring current makes the dominant contribution to the screening of the protons. An aromaticity scale was devised on the basis of the  $\pi$ -electron contribution to the diamagnetic susceptibility and  $\pi$ -electron currents.

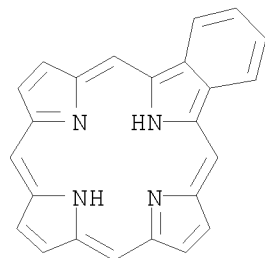
IT 36469-17-7

RL: PRP (Properties)

(NMR of, MO calcn. of)

RN 36469-17-7 CAPLUS

CN 23H,25H-Benzo[b]porphine (9CI) (CA INDEX NAME)



L9 ANSWER 101 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1981:539063 CAPLUS

DOCUMENT NUMBER: 95:139063

ORIGINAL REFERENCE NO.: 95:23181a,23184a

TITLE:  $\pi$ -Electron ring currents and magnetic properties of porphyrin molecules in the MO LCAO SCF method

AUTHOR(S): Vysotskii, Yu. B.; Kuz'mitskii, V. A.; Solov'ev, K. N.

CORPORATE SOURCE: Inst. Phys.-Org. Chem. Coal Chem., Donetsk, 340048, USSR

SOURCE: Theoretica Chimica Acta (1981), 59(5), 467-85

CODEN: TCHAAM; ISSN: 0040-5744

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The coupled variant of double-parameter perturbation theory in the MO LCAO SCF method in the London approximation was used for the calcn. of  $\pi$ -electron current distributions in the mols. of porphin and its derivs. The chemical shifts of <sup>1</sup>H-NMR were computed on the basis of calcns. of ring currents and charge distributions. It is shown that  $\pi$ -electron ring currents are responsible for the dominant contribution to the shielding of protons. The theor. and exptl. values of proton chemical shifts are in a good

agreement. Chemical shifts of the  $^{13}\text{C}$  and  $^{15}\text{N}$  nuclei were also estimated. Two aromaticity scales are proposed for the compds. under study based on the calcsn. of the  $\pi$ -electron contribution to the diamagnetic susceptibility and of  $\pi$ -electron currents, resp.

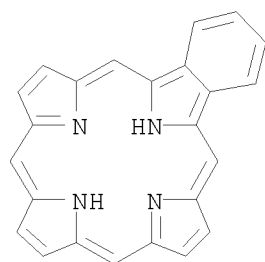
IT 36469-17-7

RL: PRP (Properties)

( $\pi$ -electron ring currents and magnetic properties of, MO LCAO SCF calcn. of)

RN 36469-17-7 CAPLUS

CN 23H,25H-Benzo[b]porphine (9CI) (CA INDEX NAME)



L9 ANSWER 102 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1978:22858 CAPLUS

DOCUMENT NUMBER: 88:22858

ORIGINAL REFERENCE NO.: 88:3673a,3676a

TITLE: The chemistry of pyrrolic compounds. XXXVII.  
Monobenzoporphyrins: the rhodoporphyrin of petroleum deposits

AUTHOR(S): Clezy, Peter S.; Fookes, Christopher J. R.; Mirza, Aminul H.

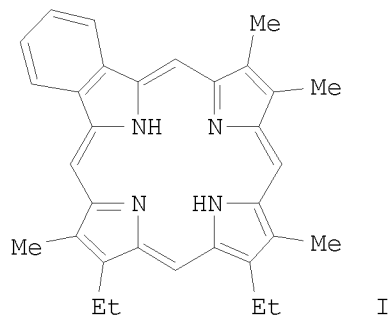
CORPORATE SOURCE: Dep. Org. Chem., Univ. New South Wales, Kensington, Australia

SOURCE: Australian Journal of Chemistry (1977), 30(6), 1337-47  
CODEN: AJCHAS; ISSN: 0004-9425

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



AB The monobenzoporphyrin I was prepared from porphyrin derivs. containing a fused

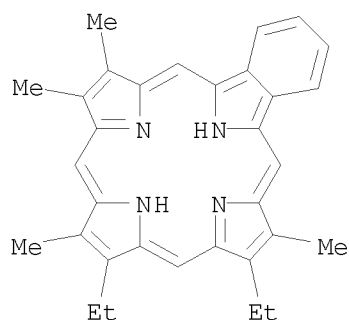
cyclohexanone ring. The cyclohexanone system can be constructed either before or after the porphyrin macrocycle was synthesized. The spectroscopic properties of the monobenzoporphyrin are described and these support the proposal that such a species constitutes the rhodo-type series of porphyrins which were isolated from some petroleum deposits.

IT 65039-01-2P 65124-67-6P 65124-68-7P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

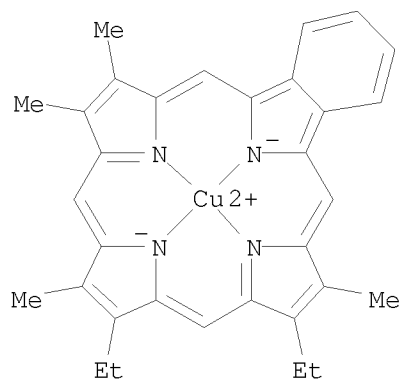
RN 65039-01-2 CAPLUS

CN 23H,25H-Benzo[b]porphine, 14,18-diethyl-8,9,13,19-tetramethyl- (9CI) (CA INDEX NAME)



RN 65124-67-6 CAPLUS

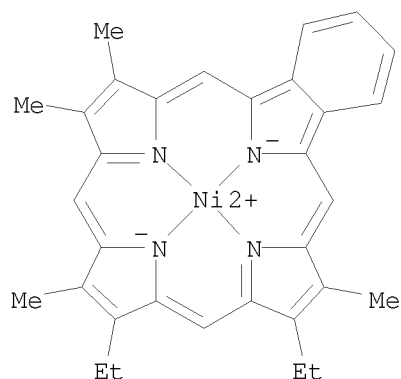
CN Copper, [9,13-diethyl-8,14,18,19-tetramethyl-23H,25H-benzo[b]porphinato(2-)-N23,N24,N25,N26]-, (SP-4-2)- (9CI) (CA INDEX NAME)



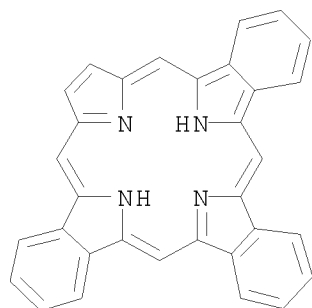
RN 65124-68-7 CAPLUS

CN Nickel, [9,13-diethyl-8,14,18,19-tetramethyl-23H,25H-benzo[b]porphinato(2-)-N23,N24,N25,N26]-, (SP-4-2)- (9CI) (CA INDEX NAME)

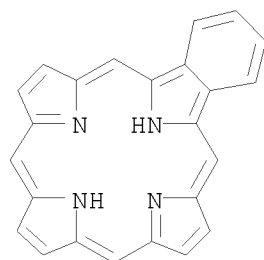




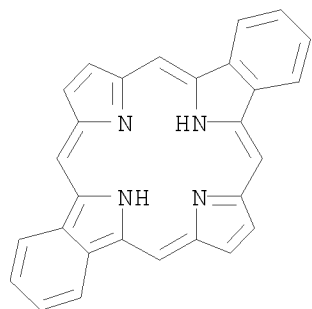
L9 ANSWER 103 OF 103 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1972:146877 CAPLUS  
 DOCUMENT NUMBER: 76:146877  
 ORIGINAL REFERENCE NO.: 76:23863a,23866a  
 TITLE: Porphyrins. XXIV. Energy, oscillator strength, and Zeeman splitting calculations [self-consistent MO configuration interaction] for phthalocyanine, porphyrins, and related ring systems  
 AUTHOR(S): McHugh, A. J.; Gouterman, Martin; Weiss, Charles, Jr.  
 CORPORATE SOURCE: Dep. Chem., Univ. Washington, Seattle, WA, USA  
 SOURCE: Theoretica Chimica Acta (1972), 24(4), 346-70  
 CODEN: TCHAAM; ISSN: 0040-5744  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Extensive CI (configuration interaction) calcns. were made on free base porphine and the metallo derivative of porphine, tetraazaporphine, phthalocyanine, various benzoporphines, chlorine, and bacteriochlorine. The transition gradient operator gives good agreement with exptl. intensities. Free base porphine may have a weak  $\pi$ - $\pi^*$  transition around 480 nm. Tetrabenzoporphine and phthalocyanine are predicted to have much more intensity around 50,000  $\text{cm}^{-1}$  than porphine and tetraazaporphine due to benzenoid transitions, a prediction borne out by the available data. Magnetic effects are calculated for the low-energy excited states. Q state angular momentum is calculated to be 4.35 .plcnst. for porphine and 3.13 .plcnst. for phthalocyanine. Although these nos. agree with some exptl. results, the calcns. show that the exptl. anal. needs further refinement.  
 IT 36469-16-6 36469-17-7 36547-73-6  
 RL: PRP (Properties)  
 (configuration interaction calcns. of, energy level, oscillator strength and Zeeman effect in relation to)  
 RN 36469-16-6 CAPLUS  
 CN 27H,29H-Tribenzo[b,g,l]porphine (9CI) (CA INDEX NAME)



RN 36469-17-7 CAPLUS  
 CN 23H,25H-Benzo[b]porphine (9CI) (CA INDEX NAME)



RN 36547-73-6 CAPLUS  
 CN 25H,27H-Dibenzo[b,1]porphine (9CI) (CA INDEX NAME)



=> log h		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	561.09	1062.80
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-81.60	-102.40

SESSION WILL BE HELD FOR 120 MINUTES  
STN INTERNATIONAL SESSION SUSPENDED AT 11:03:00 ON 19 DEC 2008